Full wwPDB EM Validation Report ⓘ

May 14, 2024 – 03:04 am BST

PDB ID	:	6RW9
EMDB ID	:	EMD-10035
Title	:	Cryo-EM structure of Morganella morganii TcdA4
Authors	:	Roderer, D.; Leidreiter, F.; Gatsogiannis, C.; Meusch, D.; Benz, R.; Raunser, S.
Deposited on	:	2019-06-04
Resolution	:	3.27 Å(reported)
Based on initial model	:	1VW1

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

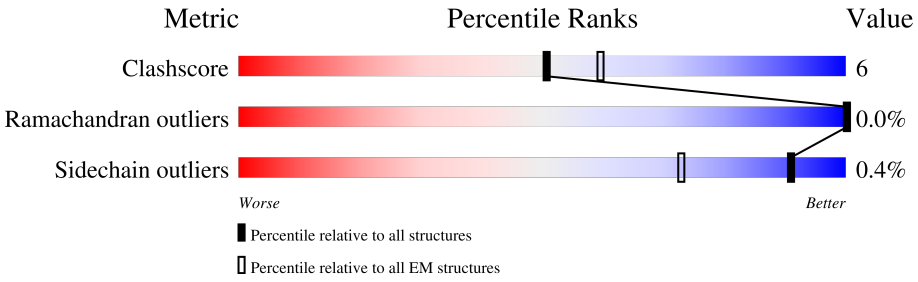
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2469	78% 14% 7%
1	B	2469	78% 14% 7%
1	C	2469	78% 14% 7%
1	D	2469	78% 15% 7%
1	E	2469	77% 15% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 88700 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Insecticidal toxin protein TcdA4.

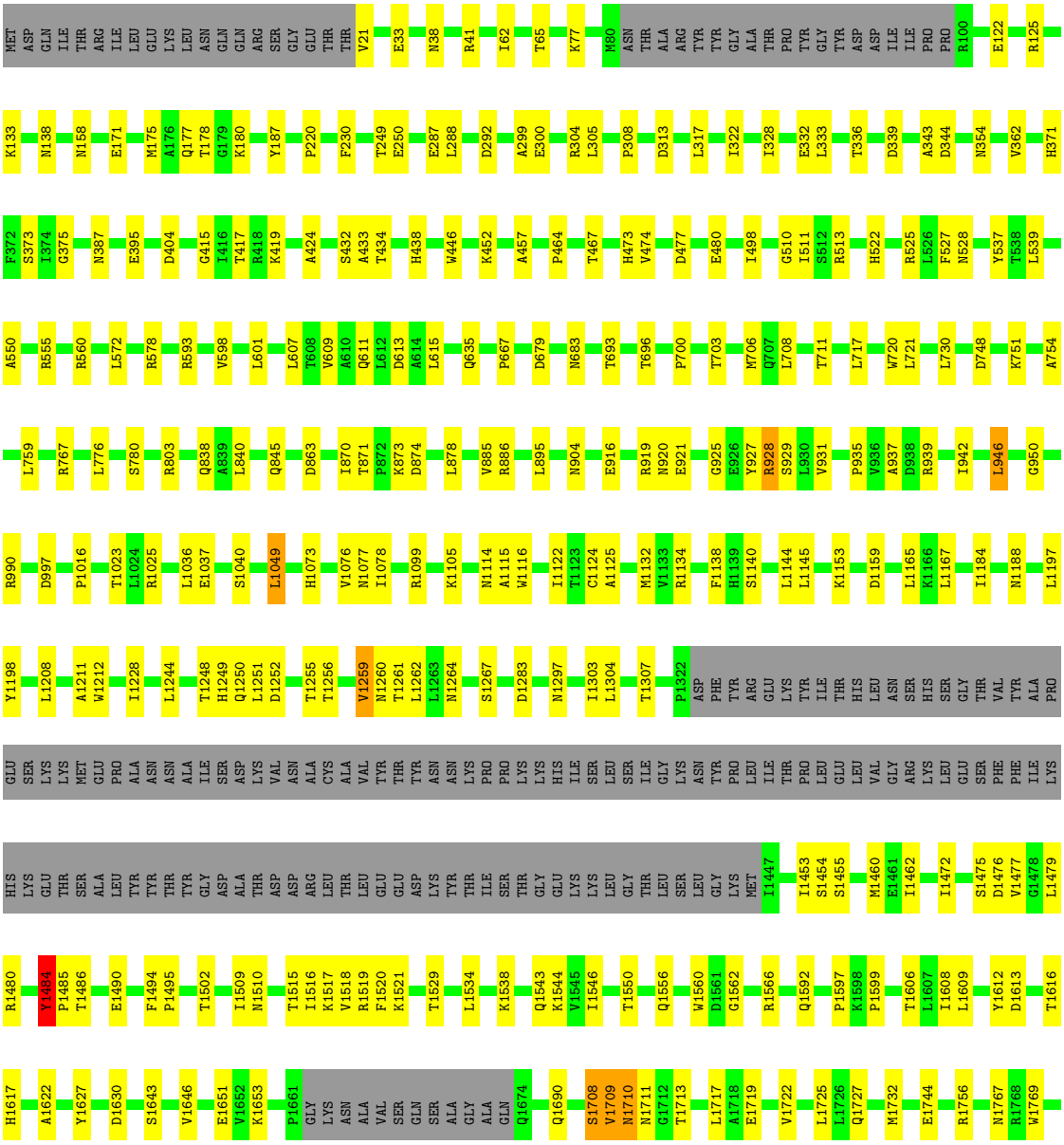
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2285	Total	C	N	O	S	0	0
			17740	11194	3070	3415	61		
1	B	2285	Total	C	N	O	S	0	0
			17740	11194	3070	3415	61		
1	C	2285	Total	C	N	O	S	0	0
			17740	11194	3070	3415	61		
1	D	2285	Total	C	N	O	S	0	0
			17740	11194	3070	3415	61		
1	E	2285	Total	C	N	O	S	0	0
			17740	11194	3070	3415	61		

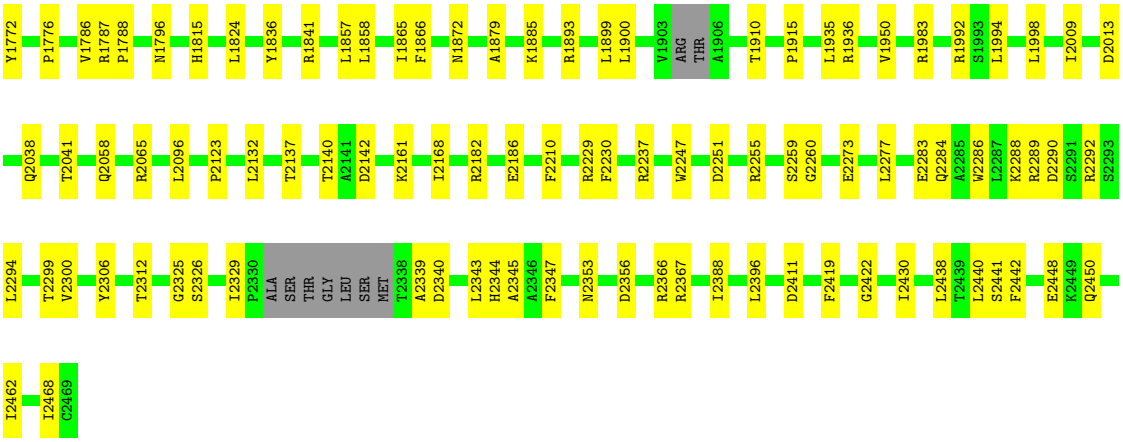
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Insecticidal toxin protein TcdA4

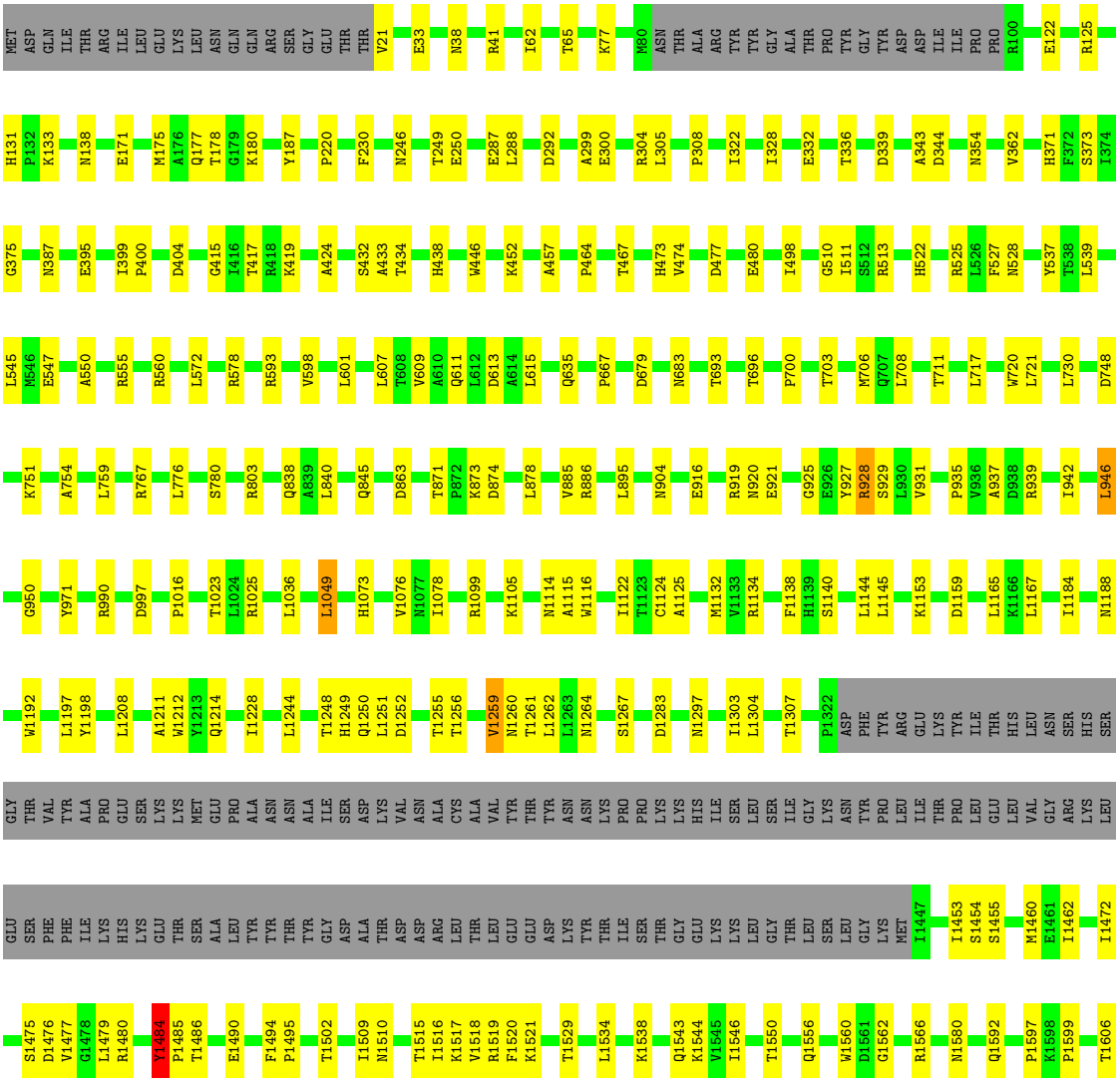
Chain A:

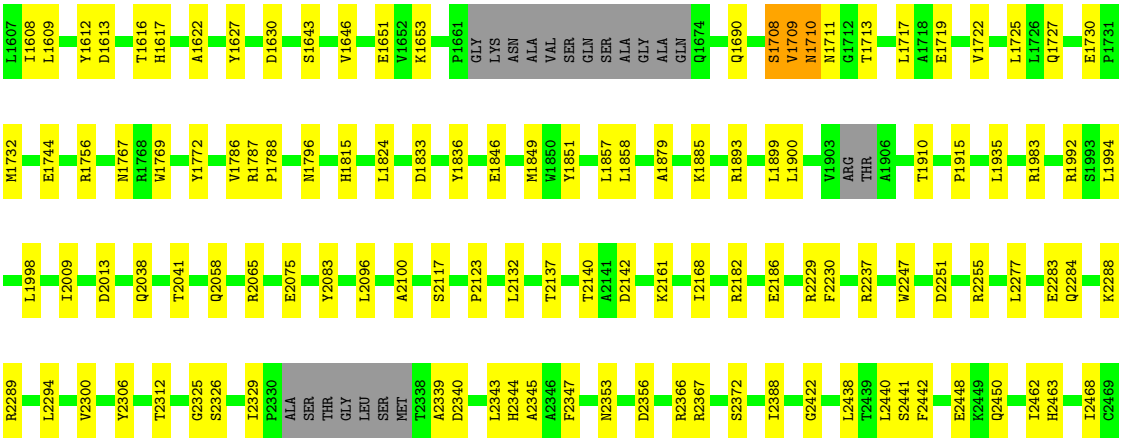




• Molecule 1: Insecticidal toxin protein TcdA4

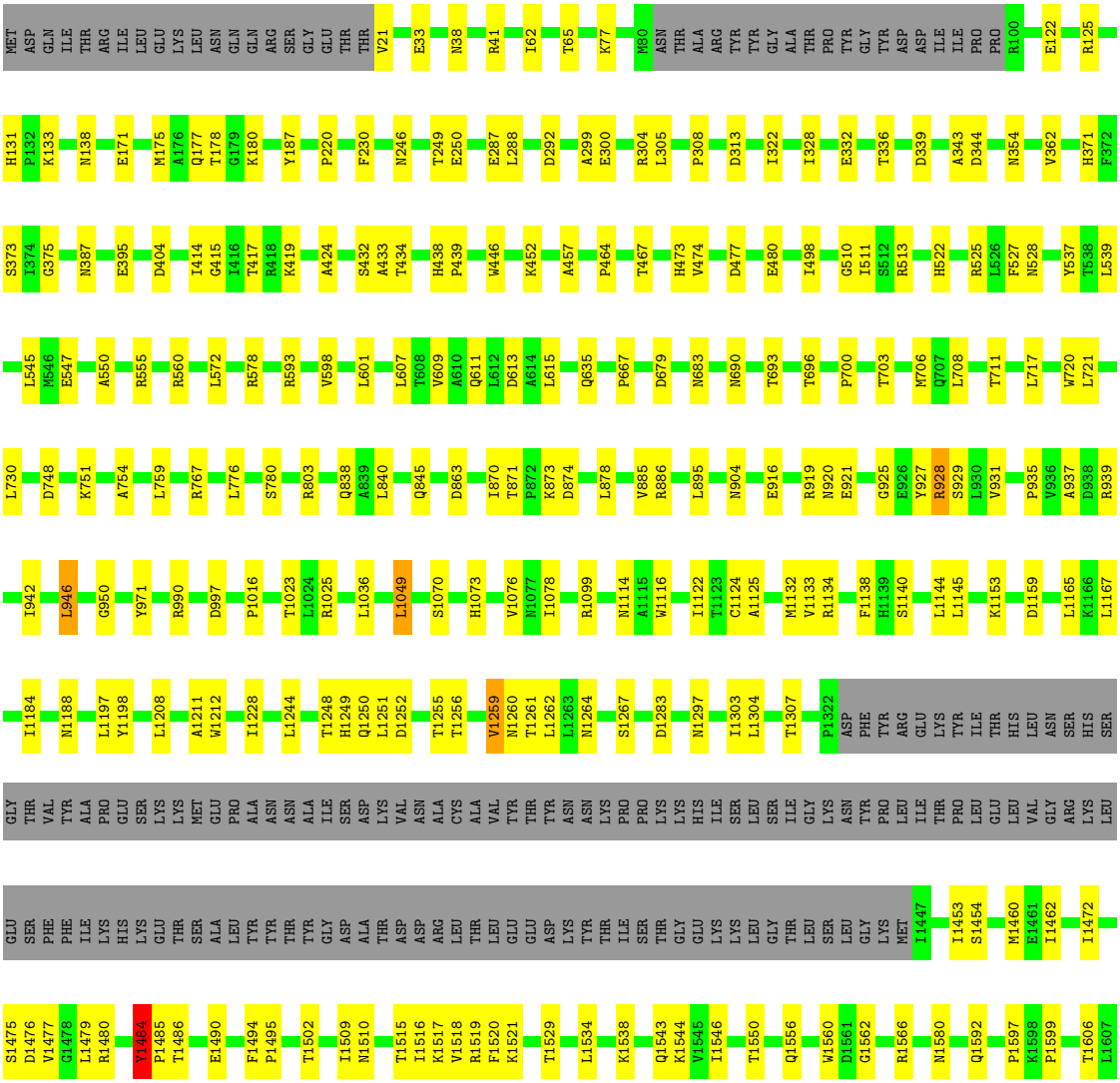
Chain B:

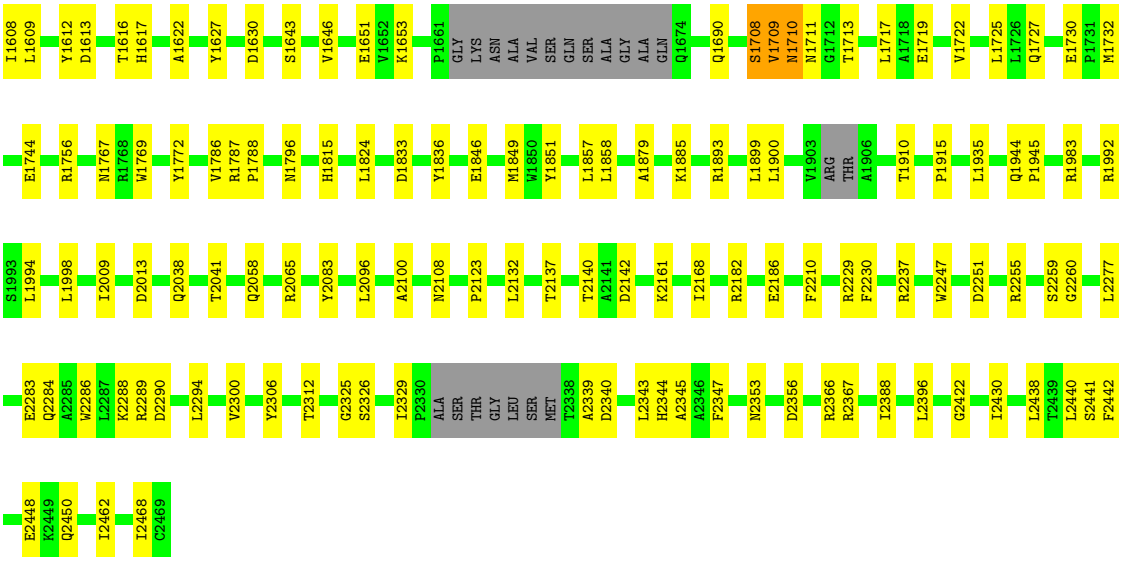




• Molecule 1: Insecticidal toxin protein TcdA4

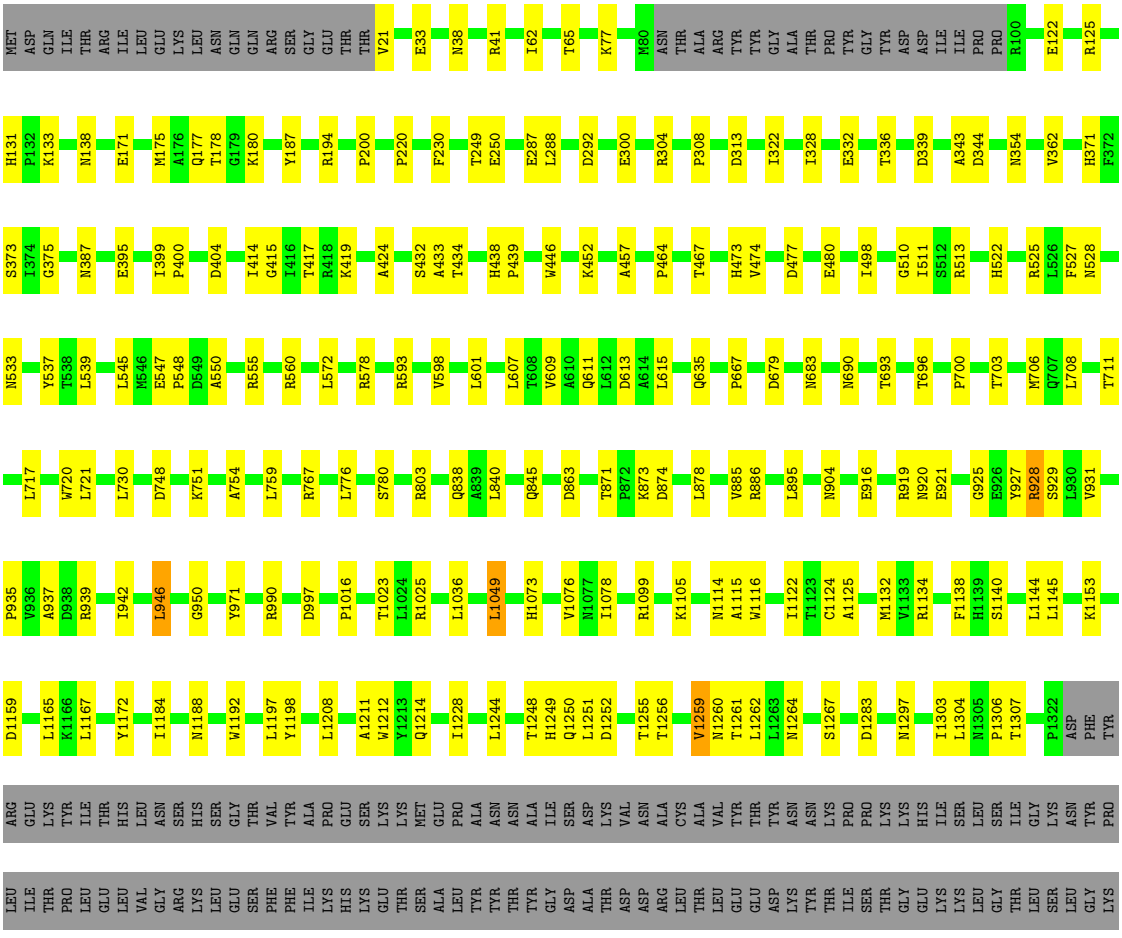
Chain C:

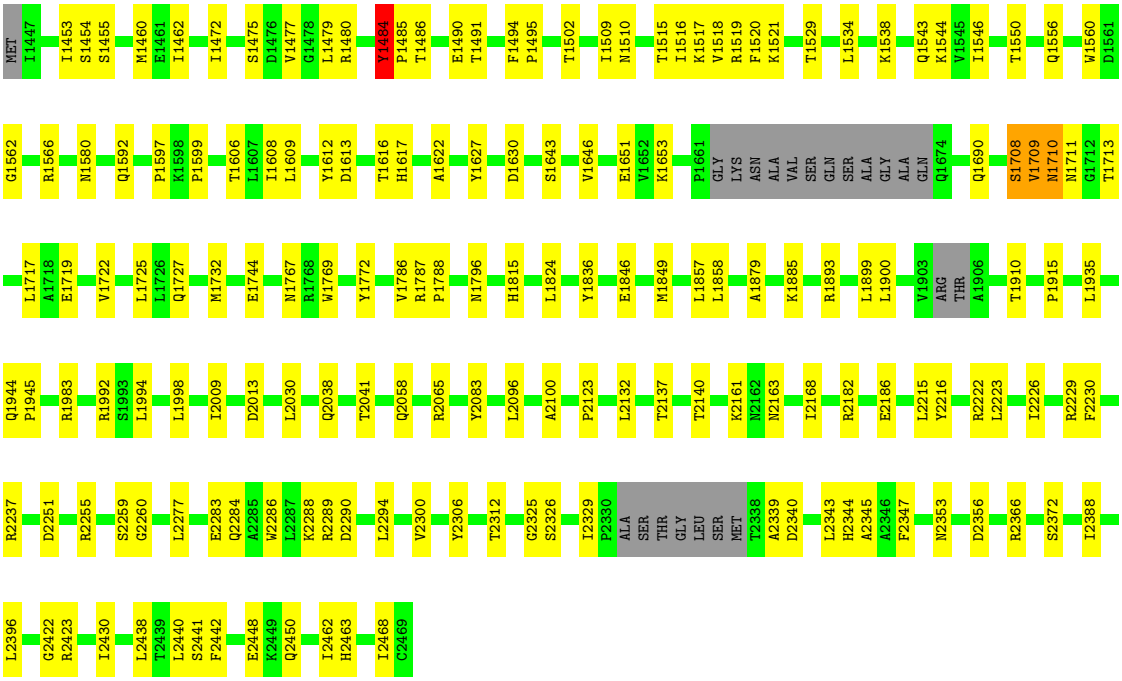




• Molecule 1: Insecticidal toxin protein TcdA4

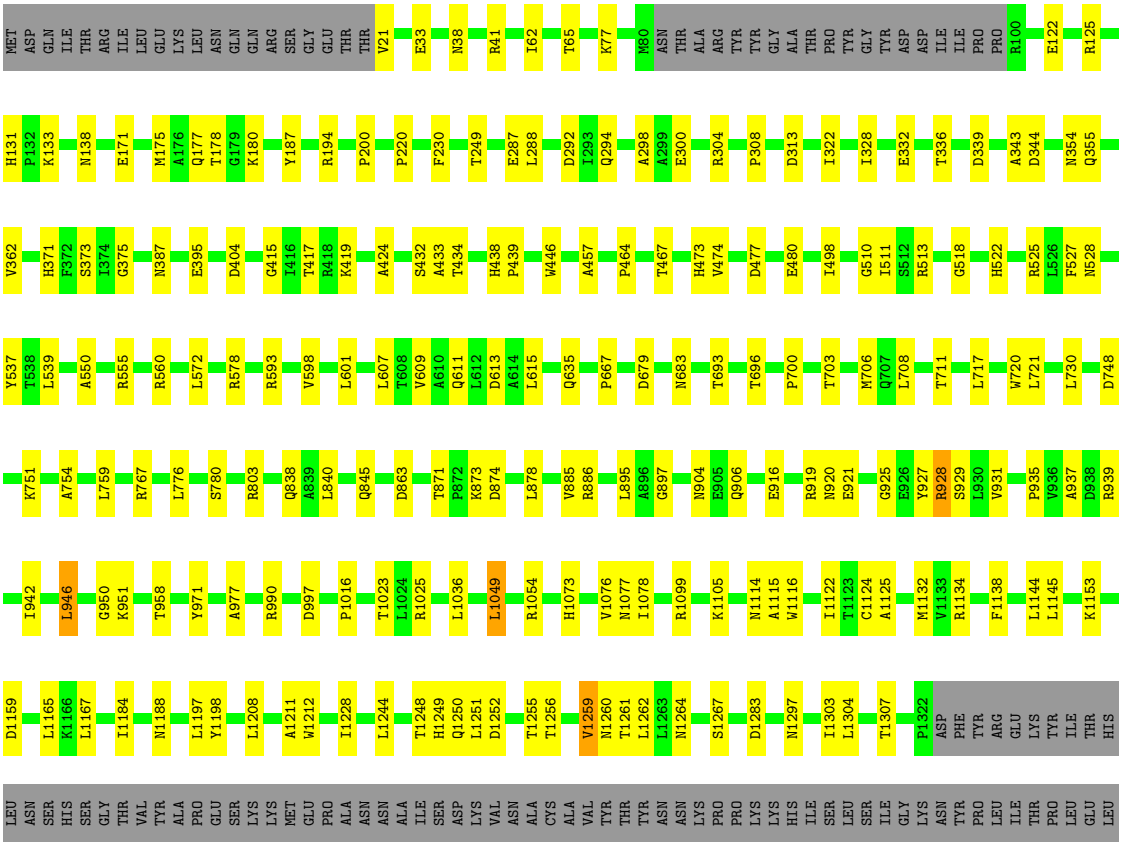
Chain D:

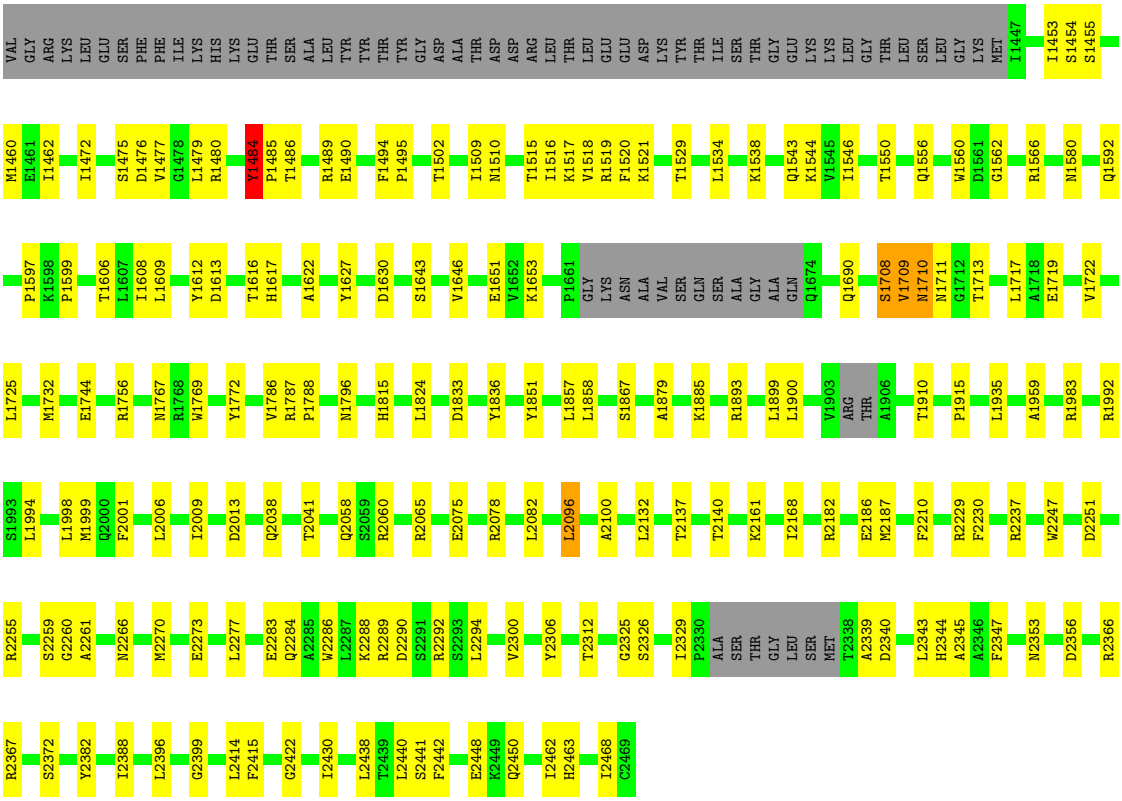




• Molecule 1: Insecticidal toxin protein TcdA4

Chain E:




VAL GLY ARG LYS LEU GLU SER PHE PHE ILE LYS HIS LYS GLU THR SER ALA LEU TYR TYR THR TYR GLY ASP ALA THR ASP ASP ARG LEU THR LEU GLU GLU ASP LYS TYR THR ILE SER THR GLY GLU LYS LYS LEU GLY THR LEU SER LEU GLY LYS MET I1447
I1453 S1454 S1455
M1460 E1461 I1462 I1472 S1475 D1476 V1477 G1478 L1479 R1480 Y1484 P1485 T1486 R1489 E1490 F1494 P1495 T1502 I1509 N1510 T1515 I1516 K1517 V1518 R1519 F1520 K1521 T1529 L1534 K1538 Q1543 K1544 V1545 I1546 T1550 Q1556 W1560 D1561 G1562 R1566 N1580 Q1592
P1597 K1598 P1599 T1606 L1607 I1608 L1609 Y1612 D1613 T1616 H1617 A1622 Y1627 D1630 S1643 V1646 E1651 V1652 K1653 P1661 GLY LYS ASN ALA VAL SER GLN SER ALA GLY ALA GLN Q1674 Q1690 S1708 V1709 N1710 N1711 G1712 T1713 L1717 A1718 E1719 V1722
L1725 M1732 E1744 R1756 N1767 R1768 W1769 Y1772 V1786 R1787 P1788 N1796 H1815 L1824 D1833 Y1836 Y1851 L1857 L1858 S1867 A1879 K1885 R1893 L1899 L1900 V1903 ARG THR A1906 T1910 P1915 L1935 A1959 R1983 R1992
S1993 L1994 L1998 M1999 Q2000 F2001 L2006 I2009 D2013 Q2038 T2041 Q2058 S2059 R2060 R2065 E2075 R2078 L2082 L2096 A2100 L2132 T2137 T2140 K2161 I2168 R2182 E2186 M2187 F2210 R2229 F2230 R2237 W2247 D2251
R2255 S2259 G2260 A2261 N2266 M2270 E2273 L2277 E2283 Q2284 A2285 W2286 L2287 K2288 R2289 D2290 S2291 R2292 S2293 L2294 V2300 Y2306 T2312 G2325 S2326 I2329 P2330 ALA SER THR GLY LEU SER MET T2338 A2339 D2340 L2343 H2344 A2345 A2346 F2347 N2353 D2356 R2366
R2367 S2372 Y2382 I2388 L2396 G2399 L2414 F2415 G2422 I2430 L2438 T2439 L2440 S2441 F2442 E2448 K2449 Q2450 I2462 H2463 I2468 C2469

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	247513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/18078	0.61	11/24569 (0.0%)
1	B	0.38	0/18078	0.61	11/24569 (0.0%)
1	C	0.38	0/18078	0.61	11/24569 (0.0%)
1	D	0.38	0/18078	0.61	11/24569 (0.0%)
1	E	0.38	0/18078	0.61	11/24569 (0.0%)
All	All	0.38	0/90390	0.61	55/122845 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
All	All	0	20

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	E	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	D	748	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	748	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	2096	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	D	2096	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	C	2096	LEU	CB-CG-CD2	-6.46	100.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	2096	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	2096	LEU	CB-CG-CD2	-6.43	100.06	111.00
1	B	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	C	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	D	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	946	LEU	CA-CB-CG	6.27	129.72	115.30
1	E	946	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	2132	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	C	2132	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	B	2132	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	D	2132	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	E	2132	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	C	1725	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	D	1725	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	E	1725	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	B	1725	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	1725	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	D	1484	TYR	C-N-CD	-5.40	108.72	120.60
1	B	1484	TYR	C-N-CD	-5.39	108.75	120.60
1	E	1484	TYR	C-N-CD	-5.38	108.76	120.60
1	C	1484	TYR	C-N-CD	-5.38	108.76	120.60
1	A	1484	TYR	C-N-CD	-5.36	108.81	120.60
1	A	1262	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	1262	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	1262	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	1262	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	1262	LEU	CA-CB-CG	5.32	127.52	115.30
1	D	840	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	E	840	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	C	1049	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	840	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	1049	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	840	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	C	840	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	E	1049	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	1049	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	1049	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	498	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	D	498	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	A	498	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	C	498	ILE	CG1-CB-CG2	-5.17	100.02	111.40
1	E	498	ILE	CG1-CB-CG2	-5.17	100.02	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2132	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	2132	LEU	CA-CB-CG	5.05	126.91	115.30
1	D	2132	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	2132	LEU	CA-CB-CG	5.04	126.88	115.30
1	E	2132	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1484	TYR	Peptide
1	A	1708	SER	Peptide
1	A	1722	VAL	Peptide
1	A	845	GLN	Peptide
1	B	1484	TYR	Peptide
1	B	1708	SER	Peptide
1	B	1722	VAL	Peptide
1	B	845	GLN	Peptide
1	C	1484	TYR	Peptide
1	C	1708	SER	Peptide
1	C	1722	VAL	Peptide
1	C	845	GLN	Peptide
1	D	1484	TYR	Peptide
1	D	1708	SER	Peptide
1	D	1722	VAL	Peptide
1	D	845	GLN	Peptide
1	E	1484	TYR	Peptide
1	E	1708	SER	Peptide
1	E	1722	VAL	Peptide
1	E	845	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17740	0	17523	224	0
1	B	17740	0	17523	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	17740	0	17523	211	0
1	D	17740	0	17523	222	0
1	E	17740	0	17523	234	0
All	All	88700	0	87615	1037	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:VAL:HG12	1:A:1788:PRO:HD2	1.72	0.72
1:C:1786:VAL:HG12	1:C:1788:PRO:HD2	1.72	0.72
1:E:1786:VAL:HG12	1:E:1788:PRO:HD2	1.72	0.71
1:B:1786:VAL:HG12	1:B:1788:PRO:HD2	1.72	0.70
1:D:1786:VAL:HG12	1:D:1788:PRO:HD2	1.72	0.70
1:C:1304:LEU:HB2	1:C:1494:PHE:HB2	1.75	0.68
1:D:1304:LEU:HB2	1:D:1494:PHE:HB2	1.75	0.68
1:A:1304:LEU:HB2	1:A:1494:PHE:HB2	1.75	0.68
1:E:1304:LEU:HB2	1:E:1494:PHE:HB2	1.75	0.67
1:B:1304:LEU:HB2	1:B:1494:PHE:HB2	1.75	0.67
1:C:230:PHE:HB3	1:C:635:GLN:HE21	1.62	0.65
1:D:1994:LEU:HD12	1:D:2237:ARG:HG3	1.80	0.64
1:E:1994:LEU:HD12	1:E:2237:ARG:HG3	1.80	0.64
1:B:2123:PRO:HB2	1:C:2100:ALA:HB2	1.80	0.64
1:A:1994:LEU:HD12	1:A:2237:ARG:HG3	1.80	0.64
1:B:1994:LEU:HD12	1:B:2237:ARG:HG3	1.80	0.64
1:C:1994:LEU:HD12	1:C:2237:ARG:HG3	1.80	0.64
1:E:1297:ASN:HD22	1:E:1502:THR:HG22	1.63	0.64
1:C:1297:ASN:HD22	1:C:1502:THR:HG22	1.64	0.63
1:D:1297:ASN:HD22	1:D:1502:THR:HG22	1.64	0.63
1:C:38:ASN:HB3	1:C:41:ARG:HB2	1.80	0.63
1:A:1297:ASN:HD22	1:A:1502:THR:HG22	1.64	0.63
1:D:230:PHE:HB3	1:D:635:GLN:HE21	1.62	0.63
1:B:1297:ASN:HD22	1:B:1502:THR:HG22	1.64	0.63
1:B:230:PHE:HB3	1:B:635:GLN:HE21	1.62	0.63
1:A:230:PHE:HB3	1:A:635:GLN:HE21	1.62	0.63
1:D:1073:HIS:HB3	1:D:1261:THR:HG22	1.81	0.62
1:E:38:ASN:HB3	1:E:41:ARG:HB2	1.80	0.62
1:E:1073:HIS:HB3	1:E:1261:THR:HG22	1.81	0.62
1:A:513:ARG:HH21	1:A:539:LEU:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLY:HA2	1:C:593:ARG:HG3	1.82	0.62
1:E:513:ARG:HH21	1:E:539:LEU:HD12	1.64	0.62
1:E:2448:GLU:HG3	1:E:2450:GLN:H	1.65	0.62
1:D:513:ARG:HH21	1:D:539:LEU:HD12	1.64	0.62
1:D:2215:LEU:HD12	1:E:2266:ASN:HD22	1.64	0.62
1:A:510:GLY:HA2	1:A:593:ARG:HG3	1.82	0.62
1:C:2123:PRO:HB2	1:D:2100:ALA:HB2	1.82	0.62
1:C:513:ARG:HH21	1:C:539:LEU:HD12	1.64	0.62
1:A:38:ASN:HB3	1:A:41:ARG:HB2	1.80	0.62
1:D:2448:GLU:HG3	1:D:2450:GLN:H	1.65	0.62
1:A:2448:GLU:HG3	1:A:2450:GLN:H	1.65	0.62
1:B:1073:HIS:HB3	1:B:1261:THR:HG22	1.81	0.62
1:E:230:PHE:HB3	1:E:635:GLN:HE21	1.62	0.62
1:A:1114:ASN:ND2	1:A:1796:ASN:OD1	2.33	0.62
1:B:1114:ASN:ND2	1:B:1796:ASN:OD1	2.33	0.62
1:D:1114:ASN:ND2	1:D:1796:ASN:OD1	2.33	0.61
1:B:510:GLY:HA2	1:B:593:ARG:HG3	1.82	0.61
1:B:38:ASN:HB3	1:B:41:ARG:HB2	1.80	0.61
1:D:38:ASN:HB3	1:D:41:ARG:HB2	1.80	0.61
1:C:1114:ASN:ND2	1:C:1796:ASN:OD1	2.33	0.61
1:D:510:GLY:HA2	1:D:593:ARG:HG3	1.82	0.61
1:A:1073:HIS:HB3	1:A:1261:THR:HG22	1.82	0.61
1:B:513:ARG:HH21	1:B:539:LEU:HD12	1.64	0.61
1:C:1073:HIS:HB3	1:C:1261:THR:HG22	1.81	0.61
1:C:2448:GLU:HG3	1:C:2450:GLN:H	1.65	0.61
1:E:1114:ASN:ND2	1:E:1796:ASN:OD1	2.33	0.61
1:B:415:GLY:HA2	1:B:432:SER:HA	1.83	0.60
1:B:1608:ILE:HG12	1:B:1651:GLU:HG2	1.83	0.60
1:C:415:GLY:HA2	1:C:432:SER:HA	1.83	0.60
1:D:1608:ILE:HG12	1:D:1651:GLU:HG2	1.83	0.60
1:E:415:GLY:HA2	1:E:432:SER:HA	1.83	0.60
1:D:131:HIS:HD1	1:D:971:TYR:HH	1.47	0.60
1:E:1608:ILE:HG12	1:E:1651:GLU:HG2	1.83	0.60
1:A:1732:MET:O	1:A:1787:ARG:NH2	2.35	0.60
1:B:2448:GLU:HG3	1:B:2450:GLN:H	1.65	0.60
1:A:1608:ILE:HG12	1:A:1651:GLU:HG2	1.83	0.60
1:B:2325:GLY:HA2	1:B:2340:ASP:HA	1.84	0.60
1:D:1732:MET:O	1:D:1787:ARG:NH2	2.35	0.60
1:C:2325:GLY:HA2	1:C:2340:ASP:HA	1.84	0.60
1:E:1732:MET:O	1:E:1787:ARG:NH2	2.35	0.60
1:C:131:HIS:HD1	1:C:971:TYR:HH	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2123:PRO:HB2	1:E:2100:ALA:HB2	1.84	0.60
1:D:2325:GLY:HA2	1:D:2340:ASP:HA	1.84	0.60
1:B:1732:MET:O	1:B:1787:ARG:NH2	2.35	0.60
1:E:510:GLY:HA2	1:E:593:ARG:HG3	1.82	0.60
1:B:131:HIS:HD1	1:B:971:TYR:HH	1.50	0.60
1:A:415:GLY:HA2	1:A:432:SER:HA	1.83	0.59
1:C:997:ASP:OD2	1:D:1767:ASN:ND2	2.35	0.59
1:C:1732:MET:O	1:C:1787:ARG:NH2	2.35	0.59
1:A:997:ASP:OD2	1:B:1767:ASN:ND2	2.35	0.59
1:A:1476:ASP:O	1:B:1727:GLN:NE2	2.35	0.59
1:A:1936:ARG:NH1	1:E:951:LYS:HD2	2.17	0.59
1:D:415:GLY:HA2	1:D:432:SER:HA	1.83	0.59
1:C:1608:ILE:HG12	1:C:1651:GLU:HG2	1.83	0.59
1:B:920:ASN:ND2	1:B:950:GLY:O	2.36	0.59
1:C:1476:ASP:O	1:D:1727:GLN:NE2	2.35	0.59
1:D:1519:ARG:HH21	1:D:1529:THR:HG21	1.68	0.59
1:E:2325:GLY:HA2	1:E:2340:ASP:HA	1.84	0.59
1:A:920:ASN:ND2	1:A:950:GLY:O	2.36	0.59
1:C:920:ASN:ND2	1:C:950:GLY:O	2.36	0.59
1:C:1519:ARG:HH21	1:C:1529:THR:HG21	1.68	0.59
1:A:2325:GLY:HA2	1:A:2340:ASP:HA	1.84	0.58
1:C:1613:ASP:H	1:C:1617:HIS:HD2	1.51	0.58
1:D:1613:ASP:H	1:D:1617:HIS:HD2	1.51	0.58
1:E:187:TYR:OH	1:E:919:ARG:NH2	2.36	0.58
1:D:920:ASN:ND2	1:D:950:GLY:O	2.36	0.58
1:A:336:THR:HG22	1:A:434:THR:H	1.68	0.58
1:C:336:THR:HG22	1:C:434:THR:H	1.68	0.58
1:D:336:THR:HG22	1:D:434:THR:H	1.68	0.58
1:E:706:MET:O	1:E:767:ARG:NH2	2.37	0.58
1:A:1992:ARG:NH2	1:A:2283:GLU:OE1	2.37	0.58
1:A:1519:ARG:HH21	1:A:1529:THR:HG21	1.68	0.58
1:B:706:MET:O	1:B:767:ARG:NH2	2.37	0.58
1:C:1992:ARG:NH2	1:C:2283:GLU:OE1	2.37	0.58
1:D:1516:ILE:HG12	1:D:1517:LYS:HG2	1.86	0.58
1:E:1519:ARG:HH21	1:E:1529:THR:HG21	1.68	0.58
1:D:1099:ARG:HH21	1:D:1116:TRP:HB3	1.69	0.58
1:E:1516:ILE:HG12	1:E:1517:LYS:HG2	1.86	0.58
1:D:2222:ARG:NH2	1:E:2261:ALA:O	2.37	0.58
1:E:920:ASN:ND2	1:E:950:GLY:O	2.36	0.58
1:A:1516:ILE:HG12	1:A:1517:LYS:HG2	1.86	0.58
1:B:1476:ASP:O	1:C:1727:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1519:ARG:HH21	1:B:1529:THR:HG21	1.68	0.58
1:B:1613:ASP:H	1:B:1617:HIS:HD2	1.51	0.58
1:D:187:TYR:OH	1:D:919:ARG:NH2	2.36	0.58
1:E:1099:ARG:HH21	1:E:1116:TRP:HB3	1.69	0.58
1:C:187:TYR:OH	1:C:919:ARG:NH2	2.36	0.58
1:A:187:TYR:OH	1:A:919:ARG:NH2	2.36	0.57
1:A:371:HIS:ND1	1:A:387:ASN:O	2.37	0.57
1:B:187:TYR:OH	1:B:919:ARG:NH2	2.36	0.57
1:D:706:MET:O	1:D:767:ARG:NH2	2.37	0.57
1:E:336:THR:HG22	1:E:434:THR:H	1.68	0.57
1:D:1025:ARG:NH2	1:D:1744:GLU:OE2	2.38	0.57
1:A:578:ARG:NH1	1:A:613:ASP:OD1	2.38	0.57
1:D:344:ASP:HB3	1:D:362:VAL:HA	1.86	0.57
1:A:706:MET:O	1:A:767:ARG:NH2	2.37	0.57
1:B:578:ARG:NH1	1:B:613:ASP:OD1	2.37	0.57
1:B:1992:ARG:NH2	1:B:2283:GLU:OE1	2.37	0.57
1:E:344:ASP:HB3	1:E:362:VAL:HA	1.86	0.57
1:E:371:HIS:ND1	1:E:387:ASN:O	2.37	0.57
1:A:1025:ARG:NH2	1:A:1744:GLU:OE2	2.38	0.57
1:A:1613:ASP:H	1:A:1617:HIS:HD2	1.51	0.57
1:A:2345:ALA:HB3	1:A:2440:LEU:HB3	1.87	0.57
1:C:1516:ILE:HG12	1:C:1517:LYS:HG2	1.86	0.57
1:E:1613:ASP:H	1:E:1617:HIS:HD2	1.51	0.57
1:B:371:HIS:ND1	1:B:387:ASN:O	2.37	0.57
1:B:1099:ARG:HH21	1:B:1116:TRP:HB3	1.69	0.57
1:B:1484:TYR:HA	1:B:1486:THR:H	1.70	0.57
1:C:578:ARG:NH1	1:C:613:ASP:OD1	2.37	0.57
1:C:706:MET:O	1:C:767:ARG:NH2	2.37	0.57
1:C:1099:ARG:HH21	1:C:1116:TRP:HB3	1.69	0.57
1:D:371:HIS:ND1	1:D:387:ASN:O	2.37	0.57
1:D:1484:TYR:HA	1:D:1486:THR:H	1.70	0.57
1:D:1992:ARG:NH2	1:D:2283:GLU:OE1	2.37	0.57
1:E:1992:ARG:NH2	1:E:2283:GLU:OE1	2.37	0.57
1:A:1767:ASN:ND2	1:E:997:ASP:OD2	2.37	0.57
1:B:336:THR:HG22	1:B:434:THR:H	1.68	0.57
1:B:1516:ILE:HG12	1:B:1517:LYS:HG2	1.86	0.57
1:E:1025:ARG:NH2	1:E:1744:GLU:OE2	2.38	0.57
1:B:344:ASP:HB3	1:B:362:VAL:HA	1.86	0.57
1:E:1484:TYR:HA	1:E:1486:THR:H	1.70	0.57
1:A:1484:TYR:HA	1:A:1486:THR:H	1.70	0.57
1:B:2366:ARG:HG2	1:B:2468:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2345:ALA:HB3	1:E:2440:LEU:HB3	1.87	0.56
1:A:1099:ARG:HH21	1:A:1116:TRP:HB3	1.69	0.56
1:A:2366:ARG:HG2	1:A:2468:ILE:HG12	1.87	0.56
1:B:997:ASP:OD2	1:C:1767:ASN:ND2	2.38	0.56
1:B:1025:ARG:NH2	1:B:1744:GLU:OE2	2.38	0.56
1:D:2366:ARG:HG2	1:D:2468:ILE:HG12	1.87	0.56
1:C:371:HIS:ND1	1:C:387:ASN:O	2.37	0.56
1:C:2345:ALA:HB3	1:C:2440:LEU:HB3	1.87	0.56
1:D:77:LYS:NZ	1:D:1858:LEU:O	2.39	0.56
1:A:77:LYS:NZ	1:A:1858:LEU:O	2.39	0.56
1:D:2345:ALA:HB3	1:D:2440:LEU:HB3	1.87	0.56
1:E:2366:ARG:HG2	1:E:2468:ILE:HG12	1.87	0.56
1:B:2345:ALA:HB3	1:B:2440:LEU:HB3	1.87	0.56
1:C:344:ASP:HB3	1:C:362:VAL:HA	1.86	0.56
1:C:1025:ARG:NH2	1:C:1744:GLU:OE2	2.38	0.56
1:C:2366:ARG:HG2	1:C:2468:ILE:HG12	1.87	0.56
1:E:308:PRO:HD2	1:E:473:HIS:H	1.71	0.56
1:D:171:GLU:OE2	1:D:919:ARG:NH2	2.39	0.56
1:E:171:GLU:OE2	1:E:919:ARG:NH2	2.39	0.56
1:A:344:ASP:HB3	1:A:362:VAL:HA	1.86	0.56
1:B:1076:VAL:HG21	1:B:1264:ASN:HD21	1.71	0.56
1:C:1244:LEU:HD22	1:C:1251:LEU:HD11	1.88	0.56
1:C:1484:TYR:HA	1:C:1486:THR:H	1.70	0.56
1:C:2343:LEU:HB3	1:C:2442:PHE:HB2	1.88	0.56
1:D:997:ASP:OD2	1:E:1767:ASN:ND2	2.39	0.56
1:B:171:GLU:OE2	1:B:919:ARG:NH2	2.39	0.56
1:C:474:VAL:HB	1:C:477:ASP:HB2	1.88	0.56
1:C:1453:ILE:HG23	1:C:1480:ARG:HH22	1.71	0.56
1:B:1566:ARG:NH2	1:B:1597:PRO:O	2.40	0.55
1:D:1453:ILE:HG23	1:D:1480:ARG:HH22	1.71	0.55
1:E:77:LYS:NZ	1:E:1858:LEU:O	2.39	0.55
1:E:578:ARG:NH1	1:E:613:ASP:OD1	2.38	0.55
1:B:77:LYS:NZ	1:B:1858:LEU:O	2.39	0.55
1:B:1453:ILE:HG23	1:B:1480:ARG:HH22	1.71	0.55
1:B:2300:VAL:HB	1:B:2462:ILE:HG22	1.89	0.55
1:C:171:GLU:OE2	1:C:919:ARG:NH2	2.39	0.55
1:C:2300:VAL:HB	1:C:2462:ILE:HG22	1.89	0.55
1:E:1453:ILE:HG23	1:E:1480:ARG:HH22	1.71	0.55
1:E:1566:ARG:NH2	1:E:1597:PRO:O	2.39	0.55
1:A:171:GLU:OE2	1:A:919:ARG:NH2	2.39	0.55
1:A:1453:ILE:HG23	1:A:1480:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2343:LEU:HB3	1:A:2442:PHE:HB2	1.88	0.55
1:C:395:GLU:OE2	1:C:513:ARG:NH2	2.40	0.55
1:D:1140:SER:HB3	1:E:1580:ASN:HD22	1.71	0.55
1:A:1566:ARG:NH2	1:A:1597:PRO:O	2.39	0.55
1:A:2277:LEU:HD21	1:E:2229:ARG:HD2	1.89	0.55
1:D:474:VAL:HB	1:D:477:ASP:HB2	1.88	0.55
1:D:572:LEU:HD12	1:D:609:VAL:HG21	1.89	0.55
1:D:2300:VAL:HB	1:D:2462:ILE:HG22	1.89	0.55
1:D:2343:LEU:HB3	1:D:2442:PHE:HB2	1.88	0.55
1:E:2300:VAL:HB	1:E:2462:ILE:HG22	1.89	0.55
1:A:308:PRO:HD2	1:A:473:HIS:H	1.71	0.55
1:A:2300:VAL:HB	1:A:2462:ILE:HG22	1.89	0.55
1:A:395:GLU:OE2	1:A:513:ARG:NH2	2.40	0.55
1:B:2294:LEU:HB2	1:B:2468:ILE:HB	1.89	0.55
1:C:77:LYS:NZ	1:C:1858:LEU:O	2.39	0.55
1:C:308:PRO:HD2	1:C:473:HIS:H	1.71	0.55
1:C:878:LEU:HA	1:C:895:LEU:HD11	1.89	0.55
1:A:1076:VAL:HG21	1:A:1264:ASN:HD21	1.71	0.55
1:B:528:ASN:HD21	1:B:537:TYR:H	1.55	0.55
1:C:528:ASN:HD21	1:C:537:TYR:H	1.55	0.55
1:C:572:LEU:HD12	1:C:609:VAL:HG21	1.89	0.55
1:C:1566:ARG:NH2	1:C:1597:PRO:O	2.39	0.55
1:C:2294:LEU:HB2	1:C:2468:ILE:HB	1.89	0.55
1:D:1566:ARG:NH2	1:D:1597:PRO:O	2.39	0.55
1:B:572:LEU:HD12	1:B:609:VAL:HG21	1.89	0.55
1:B:2343:LEU:HB3	1:B:2442:PHE:HB2	1.88	0.55
1:C:322:ILE:HG22	1:C:328:ILE:HG12	1.89	0.55
1:D:395:GLU:OE2	1:D:513:ARG:NH2	2.40	0.55
1:E:1076:VAL:HG21	1:E:1264:ASN:HD21	1.71	0.55
1:E:1244:LEU:HD22	1:E:1251:LEU:HD11	1.88	0.55
1:D:528:ASN:HD21	1:D:537:TYR:H	1.55	0.55
1:D:1244:LEU:HD22	1:D:1251:LEU:HD11	1.88	0.55
1:D:2294:LEU:HB2	1:D:2468:ILE:HB	1.89	0.55
1:A:474:VAL:HB	1:A:477:ASP:HB2	1.88	0.54
1:A:1040:SER:OG	1:E:2078:ARG:NH1	2.39	0.54
1:D:1076:VAL:HG21	1:D:1264:ASN:HD21	1.71	0.54
1:E:528:ASN:HD21	1:E:537:TYR:H	1.55	0.54
1:E:572:LEU:HD12	1:E:609:VAL:HG21	1.89	0.54
1:B:474:VAL:HB	1:B:477:ASP:HB2	1.88	0.54
1:E:395:GLU:OE2	1:E:513:ARG:NH2	2.40	0.54
1:E:878:LEU:HA	1:E:895:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HD13	1:A:759:LEU:HD23	1.90	0.54
1:B:1244:LEU:HD22	1:B:1251:LEU:HD11	1.88	0.54
1:C:1076:VAL:HG21	1:C:1264:ASN:HD21	1.71	0.54
1:B:721:LEU:HD13	1:B:759:LEU:HD23	1.90	0.54
1:D:322:ILE:HG22	1:D:328:ILE:HG12	1.90	0.54
1:E:474:VAL:HB	1:E:477:ASP:HB2	1.88	0.54
1:A:528:ASN:HD21	1:A:537:TYR:H	1.55	0.54
1:A:878:LEU:HA	1:A:895:LEU:HD11	1.89	0.54
1:B:322:ILE:HG22	1:B:328:ILE:HG12	1.89	0.54
1:B:395:GLU:OE2	1:B:513:ARG:NH2	2.40	0.54
1:E:928:ARG:NH1	1:E:937:ALA:O	2.41	0.54
1:A:1244:LEU:HD22	1:A:1251:LEU:HD11	1.88	0.54
1:C:721:LEU:HD13	1:C:759:LEU:HD23	1.90	0.54
1:D:928:ARG:NH1	1:D:937:ALA:O	2.41	0.54
1:D:871:THR:HG22	1:D:874:ASP:HB2	1.90	0.54
1:D:878:LEU:HA	1:D:895:LEU:HD11	1.89	0.54
1:E:921:GLU:HG3	1:E:939:ARG:HH22	1.73	0.54
1:A:928:ARG:NH1	1:A:937:ALA:O	2.41	0.54
1:E:721:LEU:HD13	1:E:759:LEU:HD23	1.90	0.54
1:A:322:ILE:HG22	1:A:328:ILE:HG12	1.90	0.54
1:A:1630:ASP:OD2	1:A:1690:GLN:NE2	2.41	0.54
1:A:1865:ILE:HA	1:E:294:GLN:NE2	2.23	0.54
1:B:1630:ASP:OD2	1:B:1690:GLN:NE2	2.41	0.54
1:B:308:PRO:HD2	1:B:473:HIS:H	1.71	0.54
1:B:878:LEU:HA	1:B:895:LEU:HD11	1.89	0.54
1:B:928:ARG:NH1	1:B:937:ALA:O	2.41	0.54
1:C:871:THR:HG22	1:C:874:ASP:HB2	1.90	0.54
1:D:308:PRO:HD2	1:D:473:HIS:H	1.71	0.54
1:A:572:LEU:HD12	1:A:609:VAL:HG21	1.89	0.53
1:A:2294:LEU:HB2	1:A:2468:ILE:HB	1.89	0.53
1:C:1630:ASP:OD2	1:C:1690:GLN:NE2	2.41	0.53
1:E:871:THR:HG22	1:E:874:ASP:HB2	1.90	0.53
1:E:2343:LEU:HB3	1:E:2442:PHE:HB2	1.88	0.53
1:A:158:ASN:ND2	1:E:518:GLY:O	2.41	0.53
1:D:721:LEU:HD13	1:D:759:LEU:HD23	1.90	0.53
1:D:1134:ARG:NH2	1:D:1252:ASP:OD2	2.41	0.53
1:E:322:ILE:HG22	1:E:328:ILE:HG12	1.89	0.53
1:E:942:ILE:O	1:E:946:LEU:HB3	2.09	0.53
1:B:871:THR:HG22	1:B:874:ASP:HB2	1.90	0.53
1:C:928:ARG:NH1	1:C:937:ALA:O	2.41	0.53
1:E:1078:ILE:HG12	1:E:1544:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2294:LEU:HB2	1:E:2468:ILE:HB	1.89	0.53
1:A:1134:ARG:NH2	1:A:1252:ASP:OD2	2.42	0.53
1:D:578:ARG:NH1	1:D:613:ASP:OD1	2.38	0.53
1:D:929:SER:HA	1:D:935:PRO:HG3	1.91	0.53
1:E:1134:ARG:NH2	1:E:1252:ASP:OD2	2.41	0.53
1:D:1078:ILE:HG12	1:D:1544:LYS:HD3	1.91	0.53
1:C:1134:ARG:NH2	1:C:1252:ASP:OD2	2.41	0.53
1:D:1630:ASP:OD2	1:D:1690:GLN:NE2	2.41	0.53
1:A:1078:ILE:HG12	1:A:1544:LYS:HD3	1.91	0.53
1:B:1134:ARG:NH2	1:B:1252:ASP:OD2	2.41	0.53
1:E:1630:ASP:OD2	1:E:1690:GLN:NE2	2.41	0.53
1:A:942:ILE:O	1:A:946:LEU:HB3	2.09	0.53
1:C:921:GLU:HG3	1:C:939:ARG:HH22	1.73	0.53
1:C:929:SER:HA	1:C:935:PRO:HG3	1.91	0.53
1:A:921:GLU:HG3	1:A:939:ARG:HH22	1.73	0.53
1:A:2123:PRO:HB2	1:B:2100:ALA:HB2	1.90	0.53
1:C:1078:ILE:HG12	1:C:1544:LYS:HD3	1.91	0.53
1:A:871:THR:HG22	1:A:874:ASP:HB2	1.90	0.53
1:B:921:GLU:HG3	1:B:939:ARG:HH22	1.73	0.53
1:B:929:SER:HA	1:B:935:PRO:HG3	1.91	0.53
1:B:942:ILE:O	1:B:946:LEU:HB3	2.09	0.52
1:B:373:SER:HB3	1:B:417:THR:HB	1.91	0.52
1:C:122:GLU:OE1	1:C:125:ARG:NH2	2.43	0.52
1:C:2229:ARG:HD2	1:D:2277:LEU:HD21	1.91	0.52
1:D:292:ASP:HB3	1:D:464:PRO:HD2	1.92	0.52
1:D:921:GLU:HG3	1:D:939:ARG:HH22	1.73	0.52
1:D:942:ILE:O	1:D:946:LEU:HB3	2.09	0.52
1:B:1477:VAL:HG12	1:B:1479:LEU:H	1.74	0.52
1:E:550:ALA:HB3	1:E:555:ARG:HH22	1.75	0.52
1:A:929:SER:HA	1:A:935:PRO:HG3	1.91	0.52
1:A:1727:GLN:NE2	1:E:1476:ASP:O	2.43	0.52
1:B:1138:PHE:HB2	1:B:1208:LEU:HD21	1.91	0.52
1:C:942:ILE:O	1:C:946:LEU:HB3	2.09	0.52
1:D:1167:LEU:HD22	1:D:1228:ILE:HD13	1.92	0.52
1:D:1477:VAL:HG12	1:D:1479:LEU:H	1.74	0.52
1:A:1167:LEU:HD22	1:A:1228:ILE:HD13	1.92	0.52
1:B:122:GLU:OE1	1:B:125:ARG:NH2	2.43	0.52
1:C:373:SER:HB3	1:C:417:THR:HB	1.91	0.52
1:C:1167:LEU:HD22	1:C:1228:ILE:HD13	1.92	0.52
1:D:2226:ILE:HG23	1:E:2277:LEU:HD22	1.92	0.52
1:B:1078:ILE:HG12	1:B:1544:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1167:LEU:HD22	1:E:1228:ILE:HD13	1.92	0.52
1:A:550:ALA:HB3	1:A:555:ARG:HH22	1.75	0.52
1:A:1138:PHE:HB2	1:A:1208:LEU:HD21	1.91	0.52
1:C:1138:PHE:HB2	1:C:1208:LEU:HD21	1.91	0.52
1:C:1477:VAL:HG12	1:C:1479:LEU:H	1.74	0.52
1:A:1477:VAL:HG12	1:A:1479:LEU:H	1.75	0.52
1:B:1622:ALA:HA	1:B:1643:SER:HA	1.92	0.52
1:E:1250:GLN:HB3	1:E:1260:ASN:HD22	1.75	0.52
1:E:1477:VAL:HG12	1:E:1479:LEU:H	1.75	0.52
1:B:1167:LEU:HD22	1:B:1228:ILE:HD13	1.92	0.51
1:B:2137:THR:HA	1:B:2140:THR:HG22	1.93	0.51
1:D:550:ALA:HB3	1:D:555:ARG:HH22	1.75	0.51
1:D:1138:PHE:HB2	1:D:1208:LEU:HD21	1.91	0.51
1:E:929:SER:HA	1:E:935:PRO:HG3	1.91	0.51
1:B:1566:ARG:HH21	1:B:1599:PRO:HD3	1.75	0.51
1:E:122:GLU:OE1	1:E:125:ARG:NH2	2.43	0.51
1:A:373:SER:HB3	1:A:417:THR:HB	1.91	0.51
1:A:1250:GLN:HB3	1:A:1260:ASN:HD22	1.75	0.51
1:D:122:GLU:OE1	1:D:125:ARG:NH2	2.43	0.51
1:D:373:SER:HB3	1:D:417:THR:HB	1.91	0.51
1:E:1138:PHE:HB2	1:E:1208:LEU:HD21	1.91	0.51
1:B:550:ALA:HB3	1:B:555:ARG:HH22	1.75	0.51
1:C:1165:LEU:HB2	1:C:1184:ILE:HD11	1.93	0.51
1:D:1023:THR:HG23	1:D:1036:LEU:HD21	1.93	0.51
1:D:1165:LEU:HB2	1:D:1184:ILE:HD11	1.93	0.51
1:D:2223:LEU:HB2	1:E:2270:MET:HE1	1.92	0.51
1:A:2038:GLN:HG3	1:E:2187:MET:SD	2.50	0.51
1:A:2137:THR:HA	1:A:2140:THR:HG22	1.92	0.51
1:B:2388:ILE:O	1:B:2441:SER:N	2.44	0.51
1:A:927:TYR:O	1:A:931:VAL:N	2.38	0.51
1:A:1566:ARG:HH21	1:A:1599:PRO:HD3	1.75	0.51
1:C:292:ASP:HB3	1:C:464:PRO:HD2	1.92	0.51
1:C:1460:MET:HA	1:C:1520:PHE:HA	1.93	0.51
1:E:1023:THR:HG23	1:E:1036:LEU:HD21	1.93	0.51
1:C:2137:THR:HA	1:C:2140:THR:HG22	1.92	0.51
1:D:1250:GLN:HB3	1:D:1260:ASN:HD22	1.75	0.51
1:D:1566:ARG:HH21	1:D:1599:PRO:HD3	1.75	0.51
1:E:1566:ARG:HH21	1:E:1599:PRO:HD3	1.75	0.51
1:A:1023:THR:HG23	1:A:1036:LEU:HD21	1.93	0.51
1:C:550:ALA:HB3	1:C:555:ARG:HH22	1.75	0.51
1:D:2388:ILE:O	1:D:2441:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1622:ALA:HA	1:A:1643:SER:HA	1.92	0.51
1:B:1460:MET:HA	1:B:1520:PHE:HA	1.93	0.51
1:C:1023:THR:HG23	1:C:1036:LEU:HD21	1.93	0.51
1:D:2229:ARG:HD2	1:E:2277:LEU:HD21	1.93	0.51
1:E:177:GLN:HG3	1:E:931:VAL:HG22	1.93	0.51
1:A:1776:PRO:HB2	1:E:977:ALA:HA	1.93	0.51
1:C:1250:GLN:HB3	1:C:1260:ASN:HD22	1.75	0.51
1:C:1566:ARG:HH21	1:C:1599:PRO:HD3	1.75	0.51
1:C:2388:ILE:O	1:C:2441:SER:N	2.44	0.51
1:E:373:SER:HB3	1:E:417:THR:HB	1.91	0.51
1:A:122:GLU:OE1	1:A:125:ARG:NH2	2.43	0.50
1:D:177:GLN:HG3	1:D:931:VAL:HG22	1.93	0.50
1:E:1165:LEU:HB2	1:E:1184:ILE:HD11	1.93	0.50
1:A:1872:ASN:H	1:E:355:GLN:HE22	1.57	0.50
1:B:2326:SER:N	1:B:2339:ALA:O	2.44	0.50
1:A:177:GLN:HG3	1:A:931:VAL:HG22	1.93	0.50
1:B:1250:GLN:HB3	1:B:1260:ASN:HD22	1.75	0.50
1:B:2229:ARG:HD2	1:C:2277:LEU:HD21	1.94	0.50
1:C:1622:ALA:HA	1:C:1643:SER:HA	1.92	0.50
1:D:1622:ALA:HA	1:D:1643:SER:HA	1.92	0.50
1:E:2388:ILE:O	1:E:2441:SER:N	2.44	0.50
1:A:292:ASP:HB3	1:A:464:PRO:HD2	1.92	0.50
1:B:292:ASP:HB3	1:B:464:PRO:HD2	1.92	0.50
1:D:2326:SER:N	1:D:2339:ALA:O	2.44	0.50
1:E:703:THR:HG21	1:E:711:THR:HA	1.94	0.50
1:E:292:ASP:HB3	1:E:464:PRO:HD2	1.92	0.50
1:B:1023:THR:HG23	1:B:1036:LEU:HD21	1.93	0.50
1:E:1250:GLN:NE2	1:E:1261:THR:OG1	2.36	0.50
1:E:1622:ALA:HA	1:E:1643:SER:HA	1.92	0.50
1:A:703:THR:HG21	1:A:711:THR:HA	1.94	0.50
1:B:1165:LEU:HB2	1:B:1184:ILE:HD11	1.93	0.50
1:C:1122:ILE:HD13	1:C:1144:LEU:HD22	1.94	0.50
1:D:322:ILE:HG12	1:E:1867:SER:HB2	1.92	0.50
1:D:1460:MET:HA	1:D:1520:PHE:HA	1.93	0.50
1:E:2137:THR:HA	1:E:2140:THR:HG22	1.93	0.50
1:E:2326:SER:N	1:E:2339:ALA:O	2.44	0.50
1:C:1248:THR:HA	1:C:1251:LEU:HD13	1.94	0.50
1:E:1460:MET:HA	1:E:1520:PHE:HA	1.93	0.50
1:A:1460:MET:HA	1:A:1520:PHE:HA	1.93	0.50
1:A:2326:SER:N	1:A:2339:ALA:O	2.44	0.50
1:B:1562:GLY:O	1:B:1627:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2326:SER:N	1:C:2339:ALA:O	2.44	0.50
1:D:703:THR:HG21	1:D:711:THR:HA	1.94	0.50
1:A:1165:LEU:HB2	1:A:1184:ILE:HD11	1.93	0.49
1:B:1250:GLN:NE2	1:B:1261:THR:OG1	2.36	0.49
1:A:925:GLY:HA2	1:A:928:ARG:HE	1.77	0.49
1:B:611:GLN:O	1:B:615:LEU:HB2	2.12	0.49
1:C:177:GLN:HG3	1:C:931:VAL:HG22	1.93	0.49
1:C:2286:TRP:O	1:C:2290:ASP:N	2.36	0.49
1:D:2137:THR:HA	1:D:2140:THR:HG22	1.93	0.49
1:B:177:GLN:HG3	1:B:931:VAL:HG22	1.93	0.49
1:B:925:GLY:HA2	1:B:928:ARG:HE	1.77	0.49
1:C:925:GLY:HA2	1:C:928:ARG:HE	1.77	0.49
1:D:927:TYR:O	1:D:931:VAL:N	2.38	0.49
1:A:511:ILE:HG23	1:A:522:HIS:HD2	1.78	0.49
1:A:1248:THR:HA	1:A:1251:LEU:HD13	1.94	0.49
1:E:1248:THR:HA	1:E:1251:LEU:HD13	1.94	0.49
1:A:607:LEU:HD21	1:A:615:LEU:HD22	1.95	0.49
1:A:611:GLN:O	1:A:615:LEU:HB2	2.12	0.49
1:A:1756:ARG:NH1	1:E:2075:GLU:OE2	2.46	0.49
1:C:2182:ARG:NH1	1:C:2186:GLU:OE2	2.46	0.49
1:E:607:LEU:HD21	1:E:615:LEU:HD22	1.95	0.49
1:A:1122:ILE:HD13	1:A:1144:LEU:HD22	1.94	0.49
1:B:511:ILE:HG23	1:B:522:HIS:HD2	1.78	0.49
1:B:703:THR:HG21	1:B:711:THR:HA	1.94	0.49
1:C:1521:LYS:HG3	1:C:1529:THR:HB	1.95	0.49
1:D:1122:ILE:HD13	1:D:1144:LEU:HD22	1.94	0.49
1:D:1521:LYS:HG3	1:D:1529:THR:HB	1.95	0.49
1:A:700:PRO:HA	1:A:703:THR:HG22	1.95	0.49
1:A:1836:TYR:HE1	1:A:1935:LEU:HG	1.78	0.49
1:D:611:GLN:O	1:D:615:LEU:HB2	2.12	0.49
1:D:1562:GLY:O	1:D:1627:TYR:OH	2.29	0.49
1:E:1562:GLY:O	1:E:1627:TYR:OH	2.29	0.49
1:E:1836:TYR:HE1	1:E:1935:LEU:HG	1.78	0.49
1:B:1122:ILE:HD13	1:B:1144:LEU:HD22	1.94	0.49
1:B:1248:THR:HA	1:B:1251:LEU:HD13	1.94	0.49
1:E:2286:TRP:O	1:E:2290:ASP:N	2.36	0.49
1:B:700:PRO:HA	1:B:703:THR:HG22	1.95	0.49
1:C:611:GLN:O	1:C:615:LEU:HB2	2.12	0.49
1:C:2142:ASP:OD1	1:D:2083:TYR:OH	2.28	0.49
1:E:925:GLY:HA2	1:E:928:ARG:HE	1.77	0.49
1:E:1249:HIS:HB3	1:E:1543:GLN:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2326:SER:N	1:E:2340:ASP:OD1	2.46	0.49
1:A:1249:HIS:HB3	1:A:1543:GLN:HG2	1.95	0.48
1:B:1454:SER:H	1:B:1480:ARG:HH21	1.61	0.48
1:D:607:LEU:HD21	1:D:615:LEU:HD22	1.95	0.48
1:D:700:PRO:HA	1:D:703:THR:HG22	1.95	0.48
1:D:1836:TYR:HE1	1:D:1935:LEU:HG	1.77	0.48
1:D:2182:ARG:NH1	1:D:2186:GLU:OE2	2.46	0.48
1:E:611:GLN:O	1:E:615:LEU:HB2	2.12	0.48
1:C:703:THR:HG21	1:C:711:THR:HA	1.94	0.48
1:C:927:TYR:O	1:C:931:VAL:N	2.38	0.48
1:D:21:VAL:O	1:D:1885:LYS:NZ	2.46	0.48
1:D:1910:THR:HG21	1:D:1915:PRO:HD3	1.95	0.48
1:D:2123:PRO:HB3	1:E:2096:LEU:HG	1.95	0.48
1:A:1613:ASP:HB3	1:A:1616:THR:HG22	1.96	0.48
1:B:1836:TYR:HE1	1:B:1935:LEU:HG	1.78	0.48
1:D:1249:HIS:HB3	1:D:1543:GLN:HG2	1.95	0.48
1:E:1613:ASP:HB3	1:E:1616:THR:HG22	1.96	0.48
1:A:1910:THR:HG21	1:A:1915:PRO:HD3	1.96	0.48
1:A:2326:SER:N	1:A:2340:ASP:OD1	2.46	0.48
1:B:1521:LYS:HG3	1:B:1529:THR:HB	1.95	0.48
1:C:700:PRO:HA	1:C:703:THR:HG22	1.95	0.48
1:D:419:LYS:HG3	1:D:424:ALA:HB3	1.95	0.48
1:E:1122:ILE:HD13	1:E:1144:LEU:HD22	1.94	0.48
1:E:1893:ARG:HD3	1:E:1899:LEU:HD23	1.95	0.48
1:E:2247:TRP:O	1:E:2367:ARG:NH2	2.38	0.48
1:A:1454:SER:H	1:A:1480:ARG:HH21	1.61	0.48
1:B:607:LEU:HD21	1:B:615:LEU:HD22	1.95	0.48
1:E:511:ILE:HG23	1:E:522:HIS:HD2	1.78	0.48
1:E:1910:THR:HG21	1:E:1915:PRO:HD3	1.96	0.48
1:A:1145:LEU:HD12	1:A:1167:LEU:HD13	1.95	0.48
1:A:2142:ASP:OD1	1:B:2083:TYR:OH	2.27	0.48
1:A:2419:PHE:HE2	1:E:2415:PHE:HB2	1.78	0.48
1:C:21:VAL:O	1:C:1885:LYS:NZ	2.46	0.48
1:C:1910:THR:HG21	1:C:1915:PRO:HD3	1.96	0.48
1:D:250:GLU:O	1:D:452:LYS:NZ	2.40	0.48
1:E:375:GLY:N	1:E:415:GLY:O	2.47	0.48
1:A:1893:ARG:HD3	1:A:1899:LEU:HD23	1.95	0.48
1:B:375:GLY:N	1:B:415:GLY:O	2.47	0.48
1:B:1145:LEU:HD12	1:B:1167:LEU:HD13	1.95	0.48
1:B:1613:ASP:HB3	1:B:1616:THR:HG22	1.96	0.48
1:B:2182:ARG:NH1	1:B:2186:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1249:HIS:HB3	1:C:1543:GLN:HG2	1.95	0.48
1:C:1454:SER:H	1:C:1480:ARG:HH21	1.61	0.48
1:D:1248:THR:HA	1:D:1251:LEU:HD13	1.94	0.48
1:D:2229:ARG:HG3	1:E:2277:LEU:HD11	1.96	0.48
1:D:2251:ASP:OD2	1:D:2289:ARG:NH1	2.47	0.48
1:E:419:LYS:HG3	1:E:424:ALA:HB3	1.95	0.48
1:A:2182:ARG:NH1	1:A:2186:GLU:OE2	2.46	0.48
1:B:2251:ASP:OD2	1:B:2289:ARG:NH1	2.47	0.48
1:C:607:LEU:HD21	1:C:615:LEU:HD22	1.95	0.48
1:D:1613:ASP:HB3	1:D:1616:THR:HG22	1.96	0.48
1:A:1521:LYS:HG3	1:A:1529:THR:HB	1.95	0.48
1:B:21:VAL:O	1:B:1885:LYS:NZ	2.46	0.48
1:B:927:TYR:O	1:B:931:VAL:N	2.38	0.48
1:B:1249:HIS:HB3	1:B:1543:GLN:HG2	1.95	0.48
1:C:1836:TYR:HE1	1:C:1935:LEU:HG	1.78	0.48
1:D:287:GLU:OE2	1:D:928:ARG:NH2	2.47	0.48
1:E:1145:LEU:HD12	1:E:1167:LEU:HD13	1.95	0.48
1:E:1521:LYS:HG3	1:E:1529:THR:HB	1.95	0.48
1:A:1562:GLY:O	1:A:1627:TYR:OH	2.29	0.48
1:C:2247:TRP:O	1:C:2367:ARG:NH2	2.38	0.48
1:C:2326:SER:N	1:C:2340:ASP:OD1	2.46	0.48
1:D:925:GLY:HA2	1:D:928:ARG:HE	1.77	0.48
1:A:1865:ILE:HA	1:E:294:GLN:HE22	1.78	0.47
1:B:419:LYS:HG3	1:B:424:ALA:HB3	1.95	0.47
1:B:1910:THR:HG21	1:B:1915:PRO:HD3	1.96	0.47
1:C:419:LYS:HG3	1:C:424:ALA:HB3	1.95	0.47
1:D:1893:ARG:HD3	1:D:1899:LEU:HD23	1.95	0.47
1:D:2326:SER:N	1:D:2340:ASP:OD1	2.46	0.47
1:E:700:PRO:HA	1:E:703:THR:HG22	1.95	0.47
1:C:1893:ARG:HD3	1:C:1899:LEU:HD23	1.95	0.47
1:E:2182:ARG:NH1	1:E:2186:GLU:OE2	2.46	0.47
1:C:511:ILE:HG23	1:C:522:HIS:HD2	1.78	0.47
1:E:21:VAL:O	1:E:1885:LYS:NZ	2.46	0.47
1:A:21:VAL:O	1:A:1885:LYS:NZ	2.46	0.47
1:A:1132:MET:HB3	1:A:1197:LEU:HD23	1.97	0.47
1:A:1769:TRP:HA	1:A:1772:TYR:HD2	1.80	0.47
1:A:2229:ARG:HD2	1:B:2277:LEU:HD21	1.95	0.47
1:C:375:GLY:N	1:C:415:GLY:O	2.47	0.47
1:E:287:GLU:OE2	1:E:928:ARG:NH2	2.46	0.47
1:E:1198:TYR:N	1:E:1211:ALA:O	2.46	0.47
1:B:1132:MET:HB3	1:B:1197:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1893:ARG:HD3	1:B:1899:LEU:HD23	1.95	0.47
1:C:1145:LEU:HD12	1:C:1167:LEU:HD13	1.95	0.47
1:C:1198:TYR:N	1:C:1211:ALA:O	2.46	0.47
1:C:1769:TRP:HA	1:C:1772:TYR:HD2	1.80	0.47
1:D:1198:TYR:N	1:D:1211:ALA:O	2.46	0.47
1:D:2163:ASN:OD1	1:E:2060:ARG:NH1	2.43	0.47
1:E:1454:SER:H	1:E:1480:ARG:HH21	1.61	0.47
1:B:2326:SER:N	1:B:2340:ASP:OD1	2.46	0.47
1:B:2353:ASN:HB3	1:B:2356:ASP:HB2	1.97	0.47
1:E:2251:ASP:OD2	1:E:2289:ARG:NH1	2.47	0.47
1:A:158:ASN:HD21	1:E:518:GLY:HA3	1.80	0.47
1:A:419:LYS:HG3	1:A:424:ALA:HB3	1.95	0.47
1:A:1124:CYS:SG	1:A:1125:ALA:N	2.88	0.47
1:A:1592:GLN:OE1	1:A:1787:ARG:N	2.46	0.47
1:C:171:GLU:OE2	1:C:187:TYR:OH	2.30	0.47
1:D:375:GLY:N	1:D:415:GLY:O	2.47	0.47
1:D:511:ILE:HG23	1:D:522:HIS:HD2	1.78	0.47
1:D:1454:SER:H	1:D:1480:ARG:HH21	1.61	0.47
1:E:720:TRP:HB2	1:E:780:SER:HA	1.97	0.47
1:E:1769:TRP:HA	1:E:1772:TYR:HD2	1.80	0.47
1:B:1769:TRP:HA	1:B:1772:TYR:HD2	1.80	0.47
1:C:2353:ASN:HB3	1:C:2356:ASP:HB2	1.97	0.47
1:D:1612:TYR:HB3	1:D:1646:VAL:HG12	1.97	0.47
1:E:1132:MET:HB3	1:E:1197:LEU:HD23	1.97	0.47
1:A:2251:ASP:OD2	1:A:2289:ARG:NH1	2.47	0.47
1:A:287:GLU:OE2	1:A:928:ARG:NH2	2.47	0.47
1:A:375:GLY:N	1:A:415:GLY:O	2.47	0.47
1:A:720:TRP:HB2	1:A:780:SER:HA	1.97	0.47
1:C:287:GLU:OE2	1:C:928:ARG:NH2	2.47	0.47
1:C:300:GLU:OE2	1:C:446:TRP:NE1	2.37	0.47
1:C:1132:MET:HB3	1:C:1197:LEU:HD23	1.97	0.47
1:C:2251:ASP:OD2	1:C:2289:ARG:NH1	2.47	0.47
1:A:1546:ILE:HG13	1:A:1560:TRP:HB3	1.97	0.46
1:A:2299:THR:HG21	1:E:2382:TYR:HB3	1.95	0.46
1:B:354:ASN:HD22	1:B:404:ASP:HA	1.81	0.46
1:B:1717:LEU:HD12	1:B:1719:GLU:H	1.80	0.46
1:D:533:ASN:HD21	1:E:897:GLY:H	1.62	0.46
1:D:1132:MET:HB3	1:D:1197:LEU:HD23	1.97	0.46
1:D:1145:LEU:HD12	1:D:1167:LEU:HD13	1.95	0.46
1:D:1998:LEU:HD12	1:D:2230:PHE:HD2	1.80	0.46
1:E:1612:TYR:HB3	1:E:1646:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1710:ASN:HD22	1:E:1711:ASN:H	1.63	0.46
1:E:1717:LEU:HD12	1:E:1719:GLU:H	1.80	0.46
1:A:693:THR:HA	1:A:696:THR:HG22	1.98	0.46
1:A:1998:LEU:HD12	1:A:2230:PHE:HD2	1.80	0.46
1:A:2353:ASN:HB3	1:A:2356:ASP:HB2	1.97	0.46
1:B:1283:ASP:H	1:B:1307:THR:HG23	1.81	0.46
1:C:693:THR:HA	1:C:696:THR:HG22	1.97	0.46
1:C:1124:CYS:SG	1:C:1125:ALA:N	2.88	0.46
1:C:1546:ILE:HG13	1:C:1560:TRP:HB3	1.97	0.46
1:C:1998:LEU:HD12	1:C:2230:PHE:HD2	1.80	0.46
1:D:1717:LEU:HD12	1:D:1719:GLU:H	1.80	0.46
1:E:1283:ASP:H	1:E:1307:THR:HG23	1.80	0.46
1:B:693:THR:HA	1:B:696:THR:HG22	1.97	0.46
1:B:1124:CYS:SG	1:B:1125:ALA:N	2.88	0.46
1:B:1509:ILE:HA	1:B:1510:ASN:HA	1.64	0.46
1:B:1612:TYR:HB3	1:B:1646:VAL:HG12	1.97	0.46
1:C:720:TRP:HB2	1:C:780:SER:HA	1.97	0.46
1:C:1562:GLY:O	1:C:1627:TYR:OH	2.29	0.46
1:C:1613:ASP:HB3	1:C:1616:THR:HG22	1.96	0.46
1:D:1710:ASN:HD22	1:D:1711:ASN:H	1.63	0.46
1:D:2347:PHE:H	1:D:2438:LEU:H	1.63	0.46
1:A:249:THR:HG23	1:A:480:GLU:HG2	1.98	0.46
1:A:354:ASN:HD22	1:A:404:ASP:HA	1.81	0.46
1:A:1198:TYR:N	1:A:1211:ALA:O	2.46	0.46
1:A:2292:ARG:HH12	1:E:2414:LEU:HD21	1.81	0.46
1:B:249:THR:HG23	1:B:480:GLU:HG2	1.98	0.46
1:B:1998:LEU:HD12	1:B:2230:PHE:HD2	1.80	0.46
1:B:2247:TRP:O	1:B:2367:ARG:NH2	2.38	0.46
1:D:1124:CYS:SG	1:D:1125:ALA:N	2.88	0.46
1:E:249:THR:HG23	1:E:480:GLU:HG2	1.98	0.46
1:A:1250:GLN:NE2	1:A:1261:THR:OG1	2.36	0.46
1:A:1708:SER:OG	1:A:1709:VAL:N	2.49	0.46
1:A:2388:ILE:O	1:A:2441:SER:N	2.44	0.46
1:B:2347:PHE:H	1:B:2438:LEU:H	1.63	0.46
1:C:1717:LEU:HD12	1:C:1719:GLU:H	1.80	0.46
1:D:249:THR:HG23	1:D:480:GLU:HG2	1.98	0.46
1:D:720:TRP:HB2	1:D:780:SER:HA	1.97	0.46
1:D:1283:ASP:H	1:D:1307:THR:HG23	1.80	0.46
1:E:2347:PHE:H	1:E:2438:LEU:H	1.63	0.46
1:C:2347:PHE:H	1:C:2438:LEU:H	1.63	0.46
1:D:1546:ILE:HG13	1:D:1560:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:THR:HG23	1:C:480:GLU:HG2	1.98	0.46
1:C:1250:GLN:NE2	1:C:1261:THR:OG1	2.36	0.46
1:C:1708:SER:OG	1:C:1709:VAL:N	2.49	0.46
1:D:1769:TRP:HA	1:D:1772:TYR:HD2	1.80	0.46
1:E:1713:THR:HA	1:E:1717:LEU:HD21	1.98	0.46
1:A:1509:ILE:HA	1:A:1510:ASN:HA	1.64	0.46
1:A:2247:TRP:O	1:A:2367:ARG:NH2	2.38	0.46
1:C:1613:ASP:H	1:C:1617:HIS:CD2	2.33	0.46
1:E:2353:ASN:HB3	1:E:2356:ASP:HB2	1.97	0.46
1:B:171:GLU:OE2	1:B:187:TYR:OH	2.30	0.46
1:B:287:GLU:OE2	1:B:928:ARG:NH2	2.47	0.46
1:B:720:TRP:HB2	1:B:780:SER:HA	1.97	0.46
1:B:1198:TYR:N	1:B:1211:ALA:O	2.46	0.46
1:E:693:THR:HA	1:E:696:THR:HG22	1.98	0.46
1:E:1124:CYS:SG	1:E:1125:ALA:N	2.88	0.46
1:A:1612:TYR:HB3	1:A:1646:VAL:HG12	1.97	0.46
1:A:1710:ASN:HD22	1:A:1711:ASN:H	1.64	0.46
1:A:1717:LEU:HD12	1:A:1719:GLU:H	1.80	0.46
1:B:1546:ILE:HG13	1:B:1560:TRP:HB3	1.97	0.46
1:B:1708:SER:OG	1:B:1709:VAL:N	2.49	0.46
1:B:1613:ASP:H	1:B:1617:HIS:CD2	2.33	0.45
1:C:457:ALA:HA	1:C:467:THR:HG21	1.98	0.45
1:D:693:THR:HA	1:D:696:THR:HG22	1.97	0.45
1:D:1713:THR:HA	1:D:1717:LEU:HD21	1.98	0.45
1:E:1708:SER:OG	1:E:1709:VAL:N	2.49	0.45
1:B:1713:THR:HA	1:B:1717:LEU:HD21	1.98	0.45
1:E:1646:VAL:HG11	1:E:1900:LEU:HD21	1.99	0.45
1:C:354:ASN:HD22	1:C:404:ASP:HA	1.81	0.45
1:C:1612:TYR:HB3	1:C:1646:VAL:HG12	1.97	0.45
1:C:1710:ASN:HD22	1:C:1711:ASN:H	1.64	0.45
1:E:1546:ILE:HG13	1:E:1560:TRP:HB3	1.97	0.45
1:A:1713:THR:HA	1:A:1717:LEU:HD21	1.98	0.45
1:A:2038:GLN:HA	1:A:2041:THR:HG22	1.99	0.45
1:B:2306:TYR:HB3	1:B:2312:THR:HA	1.98	0.45
1:C:679:ASP:OD1	1:C:683:ASN:ND2	2.50	0.45
1:D:2353:ASN:HB3	1:D:2356:ASP:HB2	1.97	0.45
1:A:2347:PHE:H	1:A:2438:LEU:H	1.63	0.45
1:B:1140:SER:HB3	1:C:1580:ASN:HD22	1.82	0.45
1:B:1710:ASN:HD22	1:B:1711:ASN:H	1.64	0.45
1:C:1283:ASP:H	1:C:1307:THR:HG23	1.80	0.45
1:C:1646:VAL:HG11	1:C:1900:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2306:TYR:HB3	1:C:2312:THR:HA	1.98	0.45
1:D:679:ASP:OD1	1:D:683:ASN:ND2	2.50	0.45
1:D:885:VAL:HG13	1:D:886:ARG:HD2	1.99	0.45
1:D:1250:GLN:NE2	1:D:1261:THR:OG1	2.36	0.45
1:E:885:VAL:HG13	1:E:886:ARG:HD2	1.99	0.45
1:E:1998:LEU:HD12	1:E:2230:PHE:HD2	1.80	0.45
1:A:1283:ASP:H	1:A:1307:THR:HG23	1.80	0.45
1:A:2273:GLU:HG3	1:E:2001:PHE:CE1	2.52	0.45
1:B:1016:PRO:HD2	1:B:1815:HIS:CD2	2.52	0.45
1:B:1646:VAL:HG11	1:B:1900:LEU:HD21	1.99	0.45
1:D:354:ASN:HD22	1:D:404:ASP:HA	1.81	0.45
1:E:522:HIS:HA	1:E:525:ARG:HG2	1.99	0.45
1:E:2388:ILE:HB	1:E:2441:SER:HB3	1.99	0.45
1:A:528:ASN:ND2	1:A:537:TYR:H	2.14	0.45
1:A:885:VAL:HG13	1:A:886:ARG:HD2	1.99	0.45
1:B:2038:GLN:HA	1:B:2041:THR:HG22	1.99	0.45
1:C:1259:VAL:HG13	1:C:1546:ILE:HG23	1.99	0.45
1:D:457:ALA:HA	1:D:467:THR:HG21	1.98	0.45
1:D:2306:TYR:HB3	1:D:2312:THR:HA	1.98	0.45
1:A:2292:ARG:HB2	1:E:2399:GLY:C	2.37	0.45
1:A:2388:ILE:HB	1:A:2441:SER:HB3	1.99	0.45
1:B:175:MET:HA	1:B:178:THR:HG22	1.99	0.45
1:B:528:ASN:ND2	1:B:537:TYR:H	2.14	0.45
1:C:667:PRO:HB3	1:C:754:ALA:HB2	1.99	0.45
1:C:1713:THR:HA	1:C:1717:LEU:HD21	1.98	0.45
1:D:1613:ASP:H	1:D:1617:HIS:CD2	2.33	0.45
1:D:1708:SER:OG	1:D:1709:VAL:N	2.49	0.45
1:D:2216:TYR:HE1	1:E:2006:LEU:HD21	1.82	0.45
1:E:354:ASN:HD22	1:E:404:ASP:HA	1.81	0.45
1:E:528:ASN:ND2	1:E:537:TYR:H	2.14	0.45
1:A:125:ARG:HB2	1:A:1879:ALA:HB1	1.99	0.45
1:A:171:GLU:OE2	1:A:187:TYR:OH	2.30	0.45
1:A:1037:GLU:HG2	1:E:2082:LEU:HD11	1.99	0.45
1:A:2058:GLN:HA	1:A:2168:ILE:HD11	1.99	0.45
1:B:679:ASP:OD1	1:B:683:ASN:ND2	2.50	0.45
1:D:62:ILE:HA	1:D:65:THR:HG22	1.99	0.45
1:D:438:HIS:HA	1:D:439:PRO:HD3	1.84	0.45
1:D:522:HIS:HA	1:D:525:ARG:HG2	1.99	0.45
1:D:2058:GLN:HA	1:D:2168:ILE:HD11	1.99	0.45
1:E:927:TYR:O	1:E:931:VAL:N	2.38	0.45
1:A:522:HIS:HA	1:A:525:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HB2	1:D:1879:ALA:HB1	1.99	0.45
1:D:916:GLU:HA	1:D:919:ARG:HG2	1.99	0.45
1:D:1509:ILE:HA	1:D:1510:ASN:HA	1.64	0.45
1:E:679:ASP:OD1	1:E:683:ASN:ND2	2.50	0.45
1:E:803:ARG:NH2	1:E:863:ASP:OD1	2.46	0.45
1:E:1824:LEU:HD22	1:E:1857:LEU:HD11	1.99	0.45
1:E:2306:TYR:HB3	1:E:2312:THR:HA	1.98	0.45
1:A:1824:LEU:HD22	1:A:1857:LEU:HD11	1.99	0.44
1:B:125:ARG:HB2	1:B:1879:ALA:HB1	1.99	0.44
1:B:667:PRO:HB3	1:B:754:ALA:HB2	1.99	0.44
1:C:522:HIS:HA	1:C:525:ARG:HG2	1.99	0.44
1:C:1016:PRO:HD2	1:C:1815:HIS:CD2	2.52	0.44
1:D:803:ARG:NH2	1:D:863:ASP:OD1	2.46	0.44
1:D:1016:PRO:HD2	1:D:1815:HIS:CD2	2.52	0.44
1:E:708:LEU:HD11	1:E:717:LEU:HD13	2.00	0.44
1:A:175:MET:HA	1:A:178:THR:HG22	1.99	0.44
1:A:916:GLU:HA	1:A:919:ARG:HG2	1.99	0.44
1:A:1259:VAL:HG13	1:A:1546:ILE:HG23	1.99	0.44
1:A:1646:VAL:HG11	1:A:1900:LEU:HD21	1.99	0.44
1:B:2388:ILE:HB	1:B:2441:SER:HB3	1.99	0.44
1:C:62:ILE:HA	1:C:65:THR:HG22	1.99	0.44
1:C:916:GLU:HA	1:C:919:ARG:HG2	1.99	0.44
1:C:1983:ARG:N	1:C:2422:GLY:O	2.51	0.44
1:E:916:GLU:HA	1:E:919:ARG:HG2	1.99	0.44
1:C:708:LEU:HD11	1:C:717:LEU:HD13	2.00	0.44
1:D:708:LEU:HD11	1:D:717:LEU:HD13	2.00	0.44
1:D:1824:LEU:HD22	1:D:1857:LEU:HD11	1.99	0.44
1:D:2286:TRP:O	1:D:2290:ASP:N	2.36	0.44
1:A:1472:ILE:HG23	1:A:1475:SER:H	1.83	0.44
1:A:2009:ILE:HG21	1:E:2210:PHE:HD2	1.82	0.44
1:B:522:HIS:HA	1:B:525:ARG:HG2	1.99	0.44
1:B:1259:VAL:HG13	1:B:1546:ILE:HG23	1.99	0.44
1:C:1756:ARG:HA	1:C:1756:ARG:HD2	1.76	0.44
1:E:62:ILE:HA	1:E:65:THR:HG22	1.99	0.44
1:E:457:ALA:HA	1:E:467:THR:HG21	1.98	0.44
1:A:679:ASP:OD1	1:A:683:ASN:ND2	2.50	0.44
1:A:1016:PRO:HD2	1:A:1815:HIS:CD2	2.52	0.44
1:B:885:VAL:HG13	1:B:886:ARG:HD2	1.99	0.44
1:C:885:VAL:HG13	1:C:886:ARG:HD2	1.99	0.44
1:E:1833:ASP:OD1	1:E:1851:TYR:OH	2.33	0.44
1:A:776:LEU:O	1:A:780:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:ILE:HD12	1:A:1560:TRP:HB2	2.00	0.44
1:A:2306:TYR:HB3	1:A:2312:THR:HA	1.98	0.44
1:B:133:LYS:HA	1:B:138:ASN:HD22	1.83	0.44
1:B:776:LEU:O	1:B:780:SER:N	2.51	0.44
1:B:1592:GLN:OE1	1:B:1787:ARG:N	2.46	0.44
1:B:1824:LEU:HD22	1:B:1857:LEU:HD11	1.99	0.44
1:D:2038:GLN:HA	1:D:2041:THR:HG22	1.99	0.44
1:E:527:PHE:O	1:E:560:ARG:NH2	2.50	0.44
1:E:2058:GLN:HA	1:E:2168:ILE:HD11	1.99	0.44
1:A:288:LEU:HD13	1:A:464:PRO:HG3	2.00	0.44
1:B:916:GLU:HA	1:B:919:ARG:HG2	1.99	0.44
1:B:2058:GLN:HA	1:B:2168:ILE:HD11	1.99	0.44
1:D:1646:VAL:HG11	1:D:1900:LEU:HD21	1.99	0.44
1:E:667:PRO:HB3	1:E:754:ALA:HB2	1.99	0.44
1:E:776:LEU:O	1:E:780:SER:N	2.51	0.44
1:E:1592:GLN:OE1	1:E:1787:ARG:N	2.46	0.44
1:E:1613:ASP:H	1:E:1617:HIS:CD2	2.33	0.44
1:A:457:ALA:HA	1:A:467:THR:HG21	1.98	0.44
1:B:62:ILE:HA	1:B:65:THR:HG22	1.99	0.44
1:B:178:THR:HG23	1:B:180:LYS:H	1.83	0.44
1:B:1472:ILE:HG23	1:B:1475:SER:H	1.83	0.44
1:C:2038:GLN:HA	1:C:2041:THR:HG22	1.99	0.44
1:D:667:PRO:HB3	1:D:754:ALA:HB2	1.99	0.44
1:E:175:MET:HA	1:E:178:THR:HG22	1.99	0.44
1:E:1016:PRO:HD2	1:E:1815:HIS:CD2	2.52	0.44
1:E:2038:GLN:HA	1:E:2041:THR:HG22	1.99	0.44
1:A:178:THR:HG23	1:A:180:LYS:H	1.83	0.44
1:B:1078:ILE:HD12	1:B:1560:TRP:HB2	2.00	0.44
1:C:133:LYS:HA	1:C:138:ASN:HD22	1.83	0.44
1:C:178:THR:HG23	1:C:180:LYS:H	1.83	0.44
1:C:1303:ILE:HG22	1:C:1495:PRO:HA	2.00	0.44
1:D:175:MET:HA	1:D:178:THR:HG22	1.99	0.44
1:D:1983:ARG:N	1:D:2422:GLY:O	2.51	0.44
1:E:288:LEU:HD13	1:E:464:PRO:HG3	2.00	0.44
1:A:667:PRO:HB3	1:A:754:ALA:HB2	1.99	0.43
1:B:457:ALA:HA	1:B:467:THR:HG21	1.98	0.43
1:B:708:LEU:HD11	1:B:717:LEU:HD13	2.00	0.43
1:B:2065:ARG:HG2	1:B:2161:LYS:HD2	2.00	0.43
1:C:175:MET:HA	1:C:178:THR:HG22	1.99	0.43
1:C:776:LEU:O	1:C:780:SER:N	2.51	0.43
1:C:1472:ILE:HG23	1:C:1475:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:THR:HG23	1:D:180:LYS:H	1.83	0.43
1:E:1078:ILE:HD12	1:E:1560:TRP:HB2	2.00	0.43
1:A:133:LYS:HA	1:A:138:ASN:HD22	1.83	0.43
1:A:313:ASP:OD1	1:A:313:ASP:N	2.51	0.43
1:C:125:ARG:HB2	1:C:1879:ALA:HB1	1.99	0.43
1:C:1078:ILE:HD12	1:C:1560:TRP:HB2	2.00	0.43
1:C:1833:ASP:OD1	1:C:1851:TYR:OH	2.33	0.43
1:D:1303:ILE:HG22	1:D:1495:PRO:HA	2.00	0.43
1:D:1472:ILE:HG23	1:D:1475:SER:H	1.83	0.43
1:D:2388:ILE:HB	1:D:2441:SER:HB3	1.99	0.43
1:E:171:GLU:OE2	1:E:187:TYR:OH	2.30	0.43
1:E:1259:VAL:HG13	1:E:1546:ILE:HG23	1.99	0.43
1:A:708:LEU:HD11	1:A:717:LEU:HD13	2.00	0.43
1:A:942:ILE:HD12	1:A:942:ILE:HA	1.74	0.43
1:A:1613:ASP:H	1:A:1617:HIS:CD2	2.33	0.43
1:C:2065:ARG:HG2	1:C:2161:LYS:HD2	2.00	0.43
1:D:527:PHE:O	1:D:560:ARG:NH2	2.50	0.43
1:E:33:GLU:HG3	1:E:990:ARG:HH21	1.83	0.43
1:E:1159:ASP:OD1	1:E:1159:ASP:N	2.51	0.43
1:E:1472:ILE:HG23	1:E:1475:SER:H	1.83	0.43
1:A:33:GLU:HG3	1:A:990:ARG:HH21	1.83	0.43
1:C:33:GLU:HG3	1:C:990:ARG:HH21	1.83	0.43
1:C:1049:LEU:HD21	1:C:1769:TRP:HE1	1.83	0.43
1:E:178:THR:HG23	1:E:180:LYS:H	1.83	0.43
1:A:339:ASP:OD1	1:A:343:ALA:N	2.41	0.43
1:A:432:SER:OG	1:A:433:ALA:N	2.52	0.43
1:A:527:PHE:O	1:A:560:ARG:NH2	2.50	0.43
1:E:125:ARG:HB2	1:E:1879:ALA:HB1	1.99	0.43
1:E:838:GLN:HG2	1:E:873:LYS:HE3	2.00	0.43
1:A:62:ILE:HA	1:A:65:THR:HG22	1.99	0.43
1:A:598:VAL:HA	1:A:601:LEU:HD12	2.01	0.43
1:B:598:VAL:HA	1:B:601:LEU:HD12	2.01	0.43
1:B:2075:GLU:OE2	1:C:1756:ARG:NH1	2.50	0.43
1:C:730:LEU:HD21	1:C:751:LYS:HD3	2.01	0.43
1:D:33:GLU:HG3	1:D:990:ARG:HH21	1.83	0.43
1:D:776:LEU:O	1:D:780:SER:N	2.51	0.43
1:E:313:ASP:OD1	1:E:313:ASP:N	2.51	0.43
1:E:1983:ARG:N	1:E:2422:GLY:O	2.51	0.43
1:B:33:GLU:HG3	1:B:990:ARG:HH21	1.83	0.43
1:B:432:SER:OG	1:B:433:ALA:N	2.52	0.43
1:B:1159:ASP:OD1	1:B:1159:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1824:LEU:HD22	1:C:1857:LEU:HD11	1.99	0.43
1:C:2388:ILE:HB	1:C:2441:SER:HB3	1.99	0.43
1:D:133:LYS:HA	1:D:138:ASN:HD22	1.83	0.43
1:D:838:GLN:HG2	1:D:873:LYS:HE3	2.00	0.43
1:D:1172:TYR:HB3	1:E:1054:ARG:HE	1.83	0.43
1:D:1259:VAL:HG13	1:D:1546:ILE:HG23	1.99	0.43
1:A:1159:ASP:N	1:A:1159:ASP:OD1	2.51	0.43
1:A:2329:ILE:HG21	1:A:2344:HIS:HB3	2.01	0.43
1:B:838:GLN:HG2	1:B:873:LYS:HE3	2.00	0.43
1:B:2142:ASP:OD1	1:C:2083:TYR:OH	2.30	0.43
1:E:1303:ILE:HG22	1:E:1495:PRO:HA	2.00	0.43
1:A:2065:ARG:HG2	1:A:2161:LYS:HD2	2.00	0.43
1:C:432:SER:OG	1:C:433:ALA:N	2.52	0.43
1:C:527:PHE:O	1:C:560:ARG:NH2	2.50	0.43
1:C:1509:ILE:HA	1:C:1510:ASN:HA	1.64	0.43
1:D:399:ILE:HA	1:D:400:PRO:HD3	1.91	0.43
1:D:1049:LEU:HD21	1:D:1769:TRP:HE1	1.83	0.43
1:D:1078:ILE:HD12	1:D:1560:TRP:HB2	2.00	0.43
1:A:1515:THR:HB	1:A:1534:LEU:HD11	2.01	0.43
1:B:250:GLU:O	1:B:452:LYS:NZ	2.40	0.43
1:B:288:LEU:HD13	1:B:464:PRO:HG3	2.00	0.43
1:C:1140:SER:HB3	1:D:1580:ASN:HD22	1.83	0.43
1:C:2058:GLN:HA	1:C:2168:ILE:HD11	1.99	0.43
1:D:288:LEU:HD13	1:D:464:PRO:HG3	2.00	0.43
1:D:598:VAL:HA	1:D:601:LEU:HD12	2.01	0.43
1:D:1306:PRO:O	1:D:1491:THR:OG1	2.31	0.43
1:E:438:HIS:HA	1:E:439:PRO:HD3	1.84	0.43
1:E:1049:LEU:HD21	1:E:1769:TRP:HE1	1.83	0.43
1:C:528:ASN:ND2	1:C:537:TYR:H	2.14	0.42
1:E:131:HIS:ND1	1:E:971:TYR:OH	2.47	0.42
1:E:598:VAL:HA	1:E:601:LEU:HD12	2.01	0.42
1:A:332:GLU:OE2	1:A:438:HIS:NE2	2.53	0.42
1:A:803:ARG:NH2	1:A:863:ASP:OD1	2.46	0.42
1:B:131:HIS:ND1	1:B:971:TYR:OH	2.47	0.42
1:C:339:ASP:OD1	1:C:343:ALA:N	2.41	0.42
1:C:598:VAL:HA	1:C:601:LEU:HD12	2.01	0.42
1:E:133:LYS:HA	1:E:138:ASN:HD22	1.83	0.42
1:E:432:SER:OG	1:E:433:ALA:N	2.52	0.42
1:E:730:LEU:HD21	1:E:751:LYS:HD3	2.01	0.42
1:E:1509:ILE:HA	1:E:1510:ASN:HA	1.64	0.42
1:B:942:ILE:HD12	1:B:942:ILE:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:THR:HB	1:B:1534:LEU:HD11	2.01	0.42
1:C:942:ILE:HA	1:C:942:ILE:HD12	1.74	0.42
1:C:2210:PHE:HD2	1:D:2009:ILE:HG21	1.83	0.42
1:E:2329:ILE:HG21	1:E:2344:HIS:HB3	2.01	0.42
1:A:730:LEU:HD21	1:A:751:LYS:HD3	2.01	0.42
1:C:838:GLN:HG2	1:C:873:LYS:HE3	2.00	0.42
1:C:1159:ASP:N	1:C:1159:ASP:OD1	2.51	0.42
1:D:528:ASN:ND2	1:D:537:TYR:H	2.14	0.42
1:D:2065:ARG:HG2	1:D:2161:LYS:HD2	2.00	0.42
1:A:1023:THR:HG21	1:E:2078:ARG:HH21	1.85	0.42
1:A:1255:THR:HG23	1:A:1256:THR:HG23	2.01	0.42
1:B:1983:ARG:N	1:B:2422:GLY:O	2.51	0.42
1:B:2347:PHE:O	1:B:2438:LEU:N	2.49	0.42
1:C:1462:ILE:HG13	1:C:1518:VAL:HG22	2.01	0.42
1:C:1592:GLN:OE1	1:C:1787:ARG:N	2.46	0.42
1:D:432:SER:OG	1:D:433:ALA:N	2.52	0.42
1:A:220:PRO:HB2	1:A:230:PHE:CE1	2.55	0.42
1:A:1049:LEU:HD21	1:A:1769:TRP:HE1	1.83	0.42
1:A:1485:PRO:HB2	1:A:1490:GLU:HG3	2.01	0.42
1:A:2347:PHE:O	1:A:2438:LEU:N	2.49	0.42
1:B:1303:ILE:HG22	1:B:1495:PRO:HA	2.00	0.42
1:C:288:LEU:HD13	1:C:464:PRO:HG3	2.00	0.42
1:C:1255:THR:HG23	1:C:1256:THR:HG23	2.01	0.42
1:C:1606:THR:HA	1:C:1653:LYS:HA	2.02	0.42
1:D:730:LEU:HD21	1:D:751:LYS:HD3	2.01	0.42
1:D:1485:PRO:HB2	1:D:1490:GLU:HG3	2.01	0.42
1:E:1255:THR:HG23	1:E:1256:THR:HG23	2.01	0.42
1:E:2259:SER:OG	1:E:2260:GLY:N	2.53	0.42
1:A:1303:ILE:HG22	1:A:1495:PRO:HA	2.00	0.42
1:A:1950:VAL:HG13	1:E:906:GLN:HE21	1.83	0.42
1:A:2286:TRP:O	1:A:2290:ASP:N	2.36	0.42
1:B:332:GLU:OE2	1:B:438:HIS:NE2	2.53	0.42
1:B:527:PHE:O	1:B:560:ARG:NH2	2.50	0.42
1:D:2030:LEU:HD21	1:E:1959:ALA:HA	2.01	0.42
1:E:332:GLU:OE2	1:E:438:HIS:NE2	2.53	0.42
1:E:1485:PRO:HB2	1:E:1490:GLU:HG3	2.01	0.42
1:A:838:GLN:HG2	1:A:873:LYS:HE3	2.00	0.42
1:B:1255:THR:HG23	1:B:1256:THR:HG23	2.01	0.42
1:B:1485:PRO:HB2	1:B:1490:GLU:HG3	2.01	0.42
1:D:300:GLU:OE2	1:D:446:TRP:NE1	2.37	0.42
1:E:220:PRO:HB2	1:E:230:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2065:ARG:HG2	1:E:2161:LYS:HD2	2.00	0.42
1:A:1866:PHE:HD2	1:E:298:ALA:HB1	1.84	0.42
1:A:2259:SER:OG	1:A:2260:GLY:N	2.53	0.42
1:C:313:ASP:OD1	1:C:313:ASP:N	2.51	0.42
1:C:332:GLU:OE2	1:C:438:HIS:NE2	2.53	0.42
1:C:545:LEU:HD23	1:C:547:GLU:H	1.85	0.42
1:D:1462:ILE:HG13	1:D:1518:VAL:HG22	2.01	0.42
1:D:2329:ILE:HG21	1:D:2344:HIS:HB3	2.01	0.42
1:A:1462:ILE:HG13	1:A:1518:VAL:HG22	2.01	0.42
1:B:299:ALA:HB1	1:B:305:LEU:HD13	2.02	0.42
1:B:300:GLU:OE2	1:B:446:TRP:NE1	2.37	0.42
1:B:339:ASP:OD1	1:B:343:ALA:N	2.41	0.42
1:C:1153:LYS:HA	1:C:1159:ASP:HA	2.02	0.42
1:D:942:ILE:HD12	1:D:942:ILE:HA	1.74	0.42
1:E:1999:MET:HE2	1:E:2273:GLU:HA	2.02	0.42
1:B:220:PRO:HB2	1:B:230:PHE:CE1	2.55	0.41
1:B:1049:LEU:HD21	1:B:1769:TRP:HE1	1.83	0.41
1:C:803:ARG:NH2	1:C:863:ASP:OD1	2.46	0.41
1:D:690:ASN:O	1:D:693:THR:OG1	2.34	0.41
1:D:1159:ASP:OD1	1:D:1159:ASP:N	2.51	0.41
1:D:1515:THR:HB	1:D:1534:LEU:HD11	2.01	0.41
1:D:1606:THR:HA	1:D:1653:LYS:HA	2.02	0.41
1:D:2372:SER:O	1:D:2463:HIS:N	2.45	0.41
1:B:399:ILE:HA	1:B:400:PRO:HD3	1.91	0.41
1:C:1070:SER:OG	1:C:1133:VAL:O	2.27	0.41
1:C:2396:LEU:HD21	1:C:2430:ILE:HG12	2.02	0.41
1:D:1105:LYS:HB2	1:D:1115:ALA:HB2	2.02	0.41
1:E:2372:SER:O	1:E:2463:HIS:N	2.45	0.41
1:A:1841:ARG:HD2	1:E:958:THR:HA	2.01	0.41
1:A:2396:LEU:HD21	1:A:2430:ILE:HG12	2.02	0.41
1:B:730:LEU:HD21	1:B:751:LYS:HD3	2.01	0.41
1:C:2284:GLN:HE21	1:C:2288:LYS:HE3	1.85	0.41
1:C:2329:ILE:HG21	1:C:2344:HIS:HB3	2.01	0.41
1:D:545:LEU:HD23	1:D:547:GLU:H	1.85	0.41
1:D:1609:LEU:HA	1:D:1717:LEU:HA	2.03	0.41
1:E:1077:ASN:OD1	1:E:1077:ASN:N	2.54	0.41
1:E:2009:ILE:O	1:E:2013:ASP:HB2	2.20	0.41
1:A:299:ALA:HB1	1:A:305:LEU:HD13	2.02	0.41
1:A:1140:SER:HB3	1:B:1580:ASN:HD22	1.84	0.41
1:B:1550:THR:HB	1:B:1556:GLN:HG2	2.02	0.41
1:B:1756:ARG:HA	1:B:1756:ARG:HD2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1515:THR:HB	1:C:1534:LEU:HD11	2.01	0.41
1:D:1255:THR:HG23	1:D:1256:THR:HG23	2.01	0.41
1:D:1267:SER:HA	1:D:1538:LYS:HA	2.03	0.41
1:D:2423:ARG:HB3	1:E:2292:ARG:HD3	2.02	0.41
1:A:2009:ILE:O	1:A:2013:ASP:HB2	2.21	0.41
1:A:2273:GLU:HG3	1:E:2001:PHE:HE1	1.86	0.41
1:B:1153:LYS:HA	1:B:1159:ASP:HA	2.02	0.41
1:B:1267:SER:HA	1:B:1538:LYS:HA	2.03	0.41
1:B:1609:LEU:HA	1:B:1717:LEU:HA	2.03	0.41
1:B:2329:ILE:HG21	1:B:2344:HIS:HB3	2.01	0.41
1:B:2372:SER:O	1:B:2463:HIS:N	2.45	0.41
1:C:1485:PRO:HB2	1:C:1490:GLU:HG3	2.01	0.41
1:C:2009:ILE:O	1:C:2013:ASP:HB2	2.21	0.41
1:D:2347:PHE:O	1:D:2438:LEU:N	2.49	0.41
1:E:1462:ILE:HG13	1:E:1518:VAL:HG22	2.01	0.41
1:A:1267:SER:HA	1:A:1538:LYS:HA	2.03	0.41
1:A:1756:ARG:HD2	1:A:1756:ARG:HA	1.76	0.41
1:B:2284:GLN:HE21	1:B:2288:LYS:HE3	1.85	0.41
1:B:2343:LEU:O	1:B:2442:PHE:N	2.54	0.41
1:C:2259:SER:OG	1:C:2260:GLY:N	2.53	0.41
1:D:332:GLU:OE2	1:D:438:HIS:NE2	2.53	0.41
1:D:339:ASP:OD1	1:D:343:ALA:N	2.41	0.41
1:D:547:GLU:HA	1:D:548:PRO:HD3	1.94	0.41
1:D:1846:GLU:O	1:D:1849:MET:HG2	2.21	0.41
1:E:339:ASP:OD1	1:E:343:ALA:N	2.41	0.41
1:E:1197:LEU:HA	1:E:1212:TRP:HA	2.03	0.41
1:E:1267:SER:HA	1:E:1538:LYS:HA	2.03	0.41
1:E:1489:ARG:HA	1:E:1489:ARG:HD2	1.93	0.41
1:A:1197:LEU:HA	1:A:1212:TRP:HA	2.03	0.41
1:A:1606:THR:HA	1:A:1653:LYS:HA	2.02	0.41
1:B:1105:LYS:HB2	1:B:1115:ALA:HB2	2.02	0.41
1:B:1197:LEU:HA	1:B:1212:TRP:HA	2.03	0.41
1:C:1267:SER:HA	1:C:1538:LYS:HA	2.03	0.41
1:A:300:GLU:OE2	1:A:446:TRP:NE1	2.37	0.41
1:B:545:LEU:HD23	1:B:547:GLU:H	1.85	0.41
1:B:1462:ILE:HG13	1:B:1518:VAL:HG22	2.01	0.41
1:B:1606:THR:HA	1:B:1653:LYS:HA	2.02	0.41
1:C:690:ASN:O	1:C:693:THR:OG1	2.34	0.41
1:C:1197:LEU:HA	1:C:1212:TRP:HA	2.03	0.41
1:C:1944:GLN:HA	1:C:1945:PRO:HD3	1.94	0.41
1:D:2259:SER:OG	1:D:2260:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:GLU:OE2	1:E:446:TRP:NE1	2.37	0.41
1:E:1606:THR:HA	1:E:1653:LYS:HA	2.02	0.41
1:A:870:ILE:HB	1:A:874:ASP:HB3	2.03	0.41
1:A:1153:LYS:HA	1:A:1159:ASP:HA	2.02	0.41
1:A:1455:SER:OG	1:A:1480:ARG:NH1	2.54	0.41
1:A:1609:LEU:HA	1:A:1717:LEU:HA	2.03	0.41
1:A:2210:PHE:HD2	1:B:2009:ILE:HG21	1.86	0.41
1:A:2284:GLN:HE21	1:A:2288:LYS:HE3	1.86	0.41
1:B:1833:ASP:OD1	1:B:1851:TYR:OH	2.33	0.41
1:B:2009:ILE:O	1:B:2013:ASP:HB2	2.21	0.41
1:C:250:GLU:O	1:C:452:LYS:NZ	2.40	0.41
1:D:220:PRO:HB2	1:D:230:PHE:CE1	2.55	0.41
1:D:313:ASP:OD1	1:D:313:ASP:N	2.51	0.41
1:D:1592:GLN:OE1	1:D:1787:ARG:N	2.46	0.41
1:D:2284:GLN:HE21	1:D:2288:LYS:HE3	1.85	0.41
1:D:2396:LEU:HD21	1:D:2430:ILE:HG12	2.02	0.41
1:E:194:ARG:HA	1:E:200:PRO:HG3	2.03	0.41
1:E:1153:LYS:HA	1:E:1159:ASP:HA	2.02	0.41
1:E:1515:THR:HB	1:E:1534:LEU:HD11	2.01	0.41
1:E:1515:THR:H	1:E:1534:LEU:HD11	1.86	0.41
1:E:1550:THR:HB	1:E:1556:GLN:HG2	2.02	0.41
1:E:1756:ARG:HD2	1:E:1756:ARG:HA	1.76	0.41
1:E:2396:LEU:HD21	1:E:2430:ILE:HG12	2.02	0.41
1:A:1550:THR:HB	1:A:1556:GLN:HG2	2.02	0.41
1:B:1515:THR:H	1:B:1534:LEU:HD11	1.86	0.41
1:C:220:PRO:HB2	1:C:230:PHE:CE1	2.55	0.41
1:C:414:ILE:N	1:C:433:ALA:O	2.53	0.41
1:C:870:ILE:HB	1:C:874:ASP:HB3	2.03	0.41
1:D:171:GLU:OE2	1:D:187:TYR:OH	2.30	0.41
1:D:1197:LEU:HA	1:D:1212:TRP:HA	2.03	0.41
1:D:1515:THR:H	1:D:1534:LEU:HD11	1.86	0.41
1:E:1105:LYS:HB2	1:E:1115:ALA:HB2	2.02	0.41
1:E:1455:SER:OG	1:E:1480:ARG:NH1	2.54	0.41
1:A:1077:ASN:OD1	1:A:1077:ASN:N	2.54	0.40
1:B:1846:GLU:O	1:B:1849:MET:HG2	2.21	0.40
1:C:299:ALA:HB1	1:C:305:LEU:HD13	2.02	0.40
1:C:438:HIS:HA	1:C:439:PRO:HD3	1.84	0.40
1:C:1550:THR:HB	1:C:1556:GLN:HG2	2.02	0.40
1:D:1153:LYS:HA	1:D:1159:ASP:HA	2.02	0.40
1:E:2284:GLN:HE21	1:E:2288:LYS:HE3	1.85	0.40
1:A:1105:LYS:HB2	1:A:1115:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:THR:H	1:A:1534:LEU:HD11	1.86	0.40
1:B:803:ARG:NH2	1:B:863:ASP:OD1	2.46	0.40
1:B:1455:SER:OG	1:B:1480:ARG:NH1	2.54	0.40
1:D:194:ARG:HA	1:D:200:PRO:HG3	2.03	0.40
1:D:1944:GLN:HA	1:D:1945:PRO:HD3	1.94	0.40
1:D:2009:ILE:O	1:D:2013:ASP:HB2	2.21	0.40
1:A:1983:ARG:N	1:A:2422:GLY:O	2.51	0.40
1:B:246:ASN:OD1	1:B:886:ARG:NH2	2.54	0.40
1:B:1566:ARG:NH1	1:B:1730:GLU:OE2	2.55	0.40
1:C:246:ASN:OD1	1:C:886:ARG:NH2	2.54	0.40
1:C:1609:LEU:HA	1:C:1717:LEU:HA	2.03	0.40
1:A:2411:ASP:OD1	1:A:2411:ASP:N	2.53	0.40
1:B:1192:TRP:CE2	1:B:1214:GLN:HB2	2.57	0.40
1:B:2117:SER:O	1:C:2108:ASN:ND2	2.41	0.40
1:D:1192:TRP:CE2	1:D:1214:GLN:HB2	2.57	0.40
1:D:1455:SER:OG	1:D:1480:ARG:NH1	2.54	0.40
1:D:1550:THR:HB	1:D:1556:GLN:HG2	2.02	0.40
1:E:1609:LEU:HA	1:E:1717:LEU:HA	2.03	0.40
1:A:250:GLU:O	1:A:452:LYS:NZ	2.40	0.40
1:A:317:LEU:HB3	1:A:333:LEU:HB2	2.04	0.40
1:C:1566:ARG:NH1	1:C:1730:GLU:OE2	2.55	0.40
1:C:1846:GLU:O	1:C:1849:MET:HG2	2.21	0.40
1:D:414:ILE:N	1:D:433:ALA:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
1	B	2273/2469 (92%)	2120 (93%)	152 (7%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
1	D	2273/2469 (92%)	2118 (93%)	154 (7%)	1 (0%)	100	100
1	E	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
All	All	11365/12345 (92%)	10595 (93%)	765 (7%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1709	VAL
1	B	1709	VAL
1	C	1709	VAL
1	D	1709	VAL
1	E	1709	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	B	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	C	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	D	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	E	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
All	All	9430/10505 (90%)	9395 (100%)	35 (0%)	91	95

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	904	ASN
1	A	928	ARG
1	A	1188	ASN
1	A	1259	VAL

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Mol	Chain	Res	Type
1	A	1710	ASN
1	A	2255	ARG
1	B	304	ARG
1	B	904	ASN
1	B	928	ARG
1	B	1188	ASN
1	B	1259	VAL
1	B	1710	ASN
1	B	2255	ARG
1	C	304	ARG
1	C	904	ASN
1	C	928	ARG
1	C	1188	ASN
1	C	1259	VAL
1	C	1710	ASN
1	C	2255	ARG
1	D	304	ARG
1	D	904	ASN
1	D	928	ARG
1	D	1188	ASN
1	D	1259	VAL
1	D	1710	ASN
1	D	2255	ARG
1	E	304	ARG
1	E	904	ASN
1	E	928	ARG
1	E	1188	ASN
1	E	1259	VAL
1	E	1710	ASN
1	E	2255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	155	ASN
1	A	158	ASN
1	A	222	ASN
1	A	354	ASN
1	A	528	ASN
1	A	683	ASN
1	A	904	ASN

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Mol	Chain	Res	Type
1	A	1188	ASN
1	A	1222	ASN
1	A	1260	ASN
1	A	1264	ASN
1	A	1617	HIS
1	A	1710	ASN
1	A	1727	GLN
1	A	1767	ASN
1	A	1815	HIS
1	A	1883	GLN
1	A	2188	GLN
1	A	2407	HIS
1	B	38	ASN
1	B	155	ASN
1	B	158	ASN
1	B	222	ASN
1	B	354	ASN
1	B	528	ASN
1	B	683	ASN
1	B	904	ASN
1	B	1188	ASN
1	B	1222	ASN
1	B	1260	ASN
1	B	1264	ASN
1	B	1617	HIS
1	B	1710	ASN
1	B	1767	ASN
1	B	1815	HIS
1	B	1883	GLN
1	B	2188	GLN
1	B	2353	ASN
1	B	2407	HIS
1	B	2463	HIS
1	C	38	ASN
1	C	155	ASN
1	C	158	ASN
1	C	222	ASN
1	C	354	ASN
1	C	528	ASN
1	C	683	ASN
1	C	904	ASN
1	C	1188	ASN

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Mol	Chain	Res	Type
1	C	1222	ASN
1	C	1260	ASN
1	C	1264	ASN
1	C	1617	HIS
1	C	1710	ASN
1	C	1767	ASN
1	C	1815	HIS
1	C	1883	GLN
1	C	2188	GLN
1	C	2353	ASN
1	C	2407	HIS
1	C	2463	HIS
1	D	38	ASN
1	D	155	ASN
1	D	158	ASN
1	D	222	ASN
1	D	354	ASN
1	D	528	ASN
1	D	533	ASN
1	D	683	ASN
1	D	904	ASN
1	D	1188	ASN
1	D	1222	ASN
1	D	1260	ASN
1	D	1264	ASN
1	D	1617	HIS
1	D	1710	ASN
1	D	1767	ASN
1	D	1815	HIS
1	D	1883	GLN
1	D	2188	GLN
1	D	2200	GLN
1	D	2353	ASN
1	D	2407	HIS
1	D	2463	HIS
1	E	38	ASN
1	E	155	ASN
1	E	222	ASN
1	E	294	GLN
1	E	312	ASN
1	E	354	ASN
1	E	355	GLN

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Mol	Chain	Res	Type
1	E	528	ASN
1	E	683	ASN
1	E	904	ASN
1	E	1188	ASN
1	E	1222	ASN
1	E	1260	ASN
1	E	1264	ASN
1	E	1580	ASN
1	E	1617	HIS
1	E	1710	ASN
1	E	1815	HIS
1	E	1883	GLN
1	E	2188	GLN
1	E	2266	ASN
1	E	2407	HIS
1	E	2463	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10035. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.